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Abstract

This paper presents the very large eddy simulations (VLES) of a Jet-A spray reacting flow in a single element lean direct injection (LDI) injector by using the National Combustion Code (NCC) with and without invoking the Eulerian scalar DWFDF method, in which DWFDF is defined as the density weighted time filtered fine grained probability density function. The flow field is calculated by using the time filtered compressible Navier-Stokes equations (TFNS) with nonlinear subscale turbulence models, and when the Eulerian scalar DWFDF method is invoked, the energy and species mass fractions are calculated by solving the equation of DWFDF. A nonlinear subscale model for closing the convection term of the Eulerian scalar DWFDF equation is used and will be briefly described in this paper. Detailed comparisons between the results and available experimental data are carried out. Some positive findings of invoking the Eulerian scalar DWFDF method in both improving the simulation quality and maintaining economic computing cost are observed.

1.0 Introduction

Many engineering applications of large eddy simulations (LES) for internal combustor flows need to accurately account for the turbulence-chemistry interaction to facilitate a higher fidelity analysis of the design. In the conventional computational fluid dynamics (CFD) simulation methods the turbulence-chemistry interaction appears in an unclosed term that must be modeled, and its various empirical models have been proposed. The simplest one is the so called “laminar chemistry” which simply ignores the detailed effects of turbulence on the chemical reactions. However, in the DWFDF method, the chemical reaction source term in the DWFDF equation is in a closed form, therefore it can be directly calculated without any modeling, which is the unique feature of the probability density function (PDF) like approaches (Refs. 1, 2, and 3).

In this paper, we present the preliminary VLES results of a complex Jet-A (C₁₂H₂₃) spray reacting flow in a single element LDI injector. The simulation methods include both the conventional CFD method (TFNS) and an Eulerian scalar DWFDF method (Ref. 4), in which the velocity field is determined by the continuity and momentum equations of time filtered compressible Navier-Stokes equations. All simulations are done with the NCC code (Ref. 5) using the same numerical parameter setting and the same computational domain and grid resolution. In the pure TFNS simulation, all the subscale turbulent flux models, i.e., stresses, heat and species fluxes, are nonlinear models (Refs. 6 and 7). The basic equations and models are described in Section 2.0. In the Eulerian scalar DWFDF method, the convection term of scalar DWFDF contains a conditional 'mean' that needs to be modeled. Here a nonlinear model is introduced, which provides a diffusion process in the sample variable space (Refs. 3 and 8). A brief description about the scalar DWFDF equation and the model is given in Section 3.0.

At the present stage of simulations, we use a relatively simple spray injection model (i.e., prescribed droplet size and distribution) and a global five-species one-step kinetics for combustion chemistry (Ref. 9), so that we could concentrate more on the evaluation of different simulation approaches.

The main results of simulations, including both with and without invoking an Eulerian scalar DWDFD method, are described in Section 4.0. They are compared side by side to examine how much effects are produced by invoking the Eulerian scalar DWDFD method.

One of the main objectives of this study is to search for a consistent and stable VLES simulation tool for multiphase combustion flows. We require that this tool is of a rational “physics” based model and also able to produce the physically reasonable, numerically stable solution that can sustain over a very long (infinite) time period. And also, this tool should be relatively economic. It is encouraging to observe from the present simulations that the adopted Eulerian scalar DWDFD method does show the potential for improving the simulation quality and remaining an economic computing cost.

2.0 Basic Equations for TFNS Simulations

2.1 Time Filtered Turbulent Variables $\bar{\phi}(\mathbf{x}, t), \tilde{\phi}(\mathbf{x}, t)$

In the case of compressible turbulent reacting flow, we often deal with two types of time filtering: one with the density weighting, the other without the density weighting. The filtered turbulent variable without the density weighting is denoted by $\bar{\phi}(\mathbf{x}, t)$ and is defined as

$$\bar{\phi}(\mathbf{x}, t) = \int_{-\infty}^{+\infty} \phi(\mathbf{x}, t') G(t - t') dt' \quad (1)$$

where ϕ is the unfiltered turbulent variable, e.g., velocity components U_i , density ρ , pressure P , species mass fraction Φ_i and internal energy $e = \sum_{m=1}^N \Phi_m e_m$. The integration is over the entire time domain $-\infty < t' < +\infty$. $G(t - t')$ is the time filter with a constant filter width Δ_T and satisfies the following condition and asymptotic property:

$$\int_{-\infty}^{+\infty} G(t - t') dt' = 1 \quad (2)$$

$$\int_{-\infty}^{+\infty} \phi(\mathbf{x}, t') G(t - t') dt' = \phi(\mathbf{x}, t), \quad \text{as } \Delta_T \rightarrow 0 \quad (3)$$

The density-weighted filtered turbulent variable is denoted by $\tilde{\phi}(\mathbf{x}, t)$ and is defined as

$$\tilde{\phi}(\mathbf{x}, t) = \frac{\overline{\rho \phi}}{\bar{\rho}} \quad (4)$$

These filtered variables $\bar{\phi}(\mathbf{x}, t)$, $\tilde{\phi}(\mathbf{x}, t)$ mainly represent the large scale turbulence, and they are still random but contain relatively low frequency part of the turbulent motion when comparing with the unfiltered turbulent variable $\phi(\mathbf{x}, t)$.

2.2 Basic Equation

Applying the time filtering, (1) and (4), to the compressible Navier-Stokes equations, we obtain:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_j} = 0 \quad (5)$$

$$\frac{\partial \bar{\rho} \tilde{U}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{U}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\rho \nu \left(S_{ij} - \frac{1}{3} \delta_{ij} S_{kk} \right) \right) \quad (6)$$

$$\frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{e}}{\partial x_i} = -\frac{\partial \bar{q}_i}{\partial x_i} + \overline{PS_{kk}} + 2\rho \nu \left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk} \right) + \bar{Q} \quad (7)$$

$$\frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{\Phi}_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\overline{\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i}} \right) + \bar{W}_m \quad m = 1, 2, \dots, M \quad (8)$$

where

$$\bar{P} = \bar{\rho} R \sum_{m=1}^M \frac{\overline{\Phi_m T}}{w_m} = \frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\overline{\Phi_m e}}{w_m}, \text{ or } \bar{P} = \frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\overline{\Phi_m \Phi_{M+1}}}{w_m} \quad (9)$$

$$\bar{q}_i = -\kappa \frac{\partial T}{\partial x_i} - \sum_{m=1}^M \overline{\rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i}} \quad (10)$$

In the above equations, κ , ν and $\Gamma^{(m)}$ are the molecular heat conductivity, kinematic viscosity and the m -th species diffusivity. It is commonly assumed that $\Gamma^{(m)}$ is same for all species Φ_m , and w_m is the molecular weight. The h_m , T are the enthalpy of species and the temperature, Q is the radiation rate, $W_m = \rho S_m$ is the chemical production rate of the m -th species, Φ_{M+1} represents the internal energy e , R is the universal gas constant. Note that all the fuel-spray related terms are not shown in above equations for the simplicity, please see Reference 10 for the details. These equations are general; however, unlike the constant density flows, further approximations for the terms on their right hand side are required in order to complete the density weighted time filtering process. One of such approximations leads to

$$\overline{2\rho \nu \left(S_{ij} - \frac{1}{3} \delta_{ij} S_{kk} \right)} \approx \mu \left(\frac{\partial \tilde{U}_i}{\partial x_j} + \frac{\partial \tilde{U}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{U}_k}{\partial x_k} \right) \quad (11)$$

In which, we have basically neglected the variations of μ and ρ during the filtering process, the value of μ will be considered as a known function of $\bar{P}$, $\tilde{T}$, $\dots$. Other types of approximations are also possible, for example,

$$\overline{2\rho \nu \left(S_{ij} - \frac{1}{3} \delta_{ij} S_{kk} \right)} \approx \nu \left(\frac{\partial \bar{\rho} \tilde{U}_i}{\partial x_j} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{\rho} \tilde{U}_k}{\partial x_k} \right) \quad (12)$$

Similarly,

$$\bar{q}_i = -\kappa \frac{\partial T}{\partial x_i} - \sum_{m=1}^M \overline{\rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i}} \approx -\frac{\kappa}{\bar{\rho}} \frac{\partial \bar{\rho} \tilde{T}}{\partial x_i} - \sum_{m=1}^M \Gamma^{(m)} \bar{\rho} h_m \frac{\partial \tilde{\Phi}_m}{\partial x_i} \quad (13)$$

$$\overline{\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i}} \approx \Gamma^{(m)} \frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial x_i} \quad (14)$$

Where ν , κ , c and $\Gamma^{(m)}$ are considered as the known functions of $\bar{P}$, $\tilde{T}$, $\dots$. Furthermore, we introduce the dissipation rate of the subscale turbulent kinetic energy,

$$\overline{2\rho v \left(S_{ij}S_{ij} - \frac{1}{3}S_{ii}S_{kk} \right)} \equiv \bar{\rho} \tilde{\varepsilon} \quad (15)$$

Therefore, the time filtered compressible Navier-Stokes equations can be written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_j} = 0 \quad (16)$$

$$\frac{\partial \bar{\rho} \tilde{U}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{U}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[v \left(\frac{\partial \bar{\rho} \tilde{U}_i}{\partial x_j} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{\rho} \tilde{U}_k}{\partial x_k} \right) \right] \quad (17)$$

$$\frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i e}{\partial x_i} = -\frac{\partial \bar{q}_i}{\partial x_i} + \overline{PS_{kk}} + \bar{\rho} \tilde{\varepsilon} + \bar{Q} \quad (18)$$

$$\frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{\Phi}_m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial x_i} \right) + \bar{\rho} \tilde{S}_m \quad m=1,2,\dots,M \quad (19)$$

$$\bar{P} = \bar{\rho} R \sum_{m=1}^M \frac{\tilde{\Phi}_m \tilde{T}}{w_m} = \frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\tilde{\Phi}_m e}{w_m}, \text{ or } \bar{P} = \frac{\bar{\rho} R}{c_v} \sum_{m=1}^M \frac{\tilde{\Phi}_m \tilde{\Phi}_{M+1}}{w_m} \quad (20)$$

$$\bar{q}_i = -\frac{\kappa}{\bar{\rho}} \frac{\partial \bar{\rho} \tilde{T}}{\partial x_i} - \sum_{m=1}^M \bar{\rho} \Gamma^{(m)} h_m \frac{\partial \tilde{\Phi}_m}{\partial x_i} \quad (21)$$

These equations are considered quite general, because i) they are exact if the flow becomes a constant density incompressible flow, ii) all the approximations made in Equations (17), (18) and (19) are related only to the molecular diffusion terms which are less important and even become negligibly small, because they are of $O(1/\text{Re})$ comparing with the convection terms on the left hand side for turbulent flows at high Reynolds numbers (see Refs. 11 and 1). In addition, Equation (16) to (19) are often used together with the further approximations for (20) and (21):

$$\bar{P} = \bar{\rho} R \sum_{m=1}^M \frac{\tilde{\Phi}_m \tilde{T}}{w_m} = \left(\frac{\bar{\rho} R \tilde{T}}{\bar{M}} \right) \approx \frac{\bar{\rho} R \tilde{T}}{\bar{M}}, \quad \frac{1}{\bar{M}} = \sum_{m=1}^M \frac{\tilde{\Phi}_m}{w_m}, \quad \frac{1}{\bar{M}} = \sum_{m=1}^M \frac{\tilde{\Phi}_m}{w_m} \quad (22)$$

$$\bar{q}_i = -\frac{\kappa}{\bar{\rho}} \frac{\partial \bar{\rho} \tilde{T}}{\partial x_i} \quad (23)$$

The momentum flux $\bar{\rho} \tilde{U}_i \tilde{U}_j$, the energy flux $\bar{\rho} \tilde{U}_i e$ and the species flux $\bar{\rho} \tilde{U}_i \tilde{\Phi}_m$ are considered to be critically important and should be carefully modeled. Many models in the literature, from the simplest Smagorinsky model (Ref. 12) to the complex two-equation nonlinear models (Refs. 13 and 14), have been suggested in terms of subscale turbulent stresses and subscale turbulent scalar fluxes:

$\tau_{ij} \equiv \bar{\rho} (\tilde{U}_i \tilde{U}_j - \tilde{U}_i \tilde{U}_j)$ and $\Theta_i \equiv \bar{\rho} (\tilde{U}_i \tilde{\theta} - \tilde{U}_i \tilde{\theta})$, where θ represents the scalar quantities: e and Φ_m .

2.3 Nonlinear Models for Subscale Turbulent Fluxes

A general constitutive relationship between subscale turbulent stresses τ_{ij} and the strain rate of filtered turbulent flow $\tilde{S}_{ij}$, $\tilde{\Omega}_{ij}$ suggests (Ref. 15)

$$\begin{aligned}
\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = & -2f C_\mu \bar{\rho} \frac{k^2}{\varepsilon} (\tilde{S}_{ij} - \delta_{ij}\tilde{S}_{kk}/3) \\
& - A_3 f \bar{\rho} \frac{k^3}{\varepsilon^2} (\tilde{S}_{ik}\tilde{\Omega}_{kj} - \tilde{\Omega}_{ik}\tilde{S}_{kj}) \\
& + 2A_5 f \bar{\rho} \frac{k^4}{\varepsilon^3} [\tilde{\Omega}_{ik}\tilde{S}_{kj}^2 - \tilde{S}_{ik}^2\tilde{\Omega}_{kj} + \tilde{\Omega}_{ik}\tilde{S}_{km}\tilde{\Omega}_{mj} - \tilde{\Omega}_{kl}\tilde{S}_{lm}\tilde{\Omega}_{mk}\delta_{ij} + II_s(\tilde{S}_{ij} - \delta_{ij}\tilde{S}_{kk}/3)],
\end{aligned} \tag{24}$$

where, $\tilde{S}_{ij} = (\tilde{U}_{i,j} + \tilde{U}_{j,i})/2$, $\tilde{\Omega}_{ij} = (\tilde{U}_{i,j} - \tilde{U}_{j,i})/2$, $II_s = (\tilde{S}_{kk}\tilde{S}_{mm} - \tilde{S}_{kl}\tilde{S}_{lk})/2$. The model coefficients C_μ , A_3 and A_5 are constrained by the realizability condition and the rapid distortion theory limit. They are formulated as (see Ref. 14):

$$C_\mu = \frac{1}{4.0 + A_s \frac{k}{\varepsilon} U^*}, \quad A_3 = \frac{\sqrt{1.0 - A_s^2 C_\mu^2 \left(\frac{k}{\varepsilon} S^*\right)^2}}{0.5 + 1.5 \frac{k^2}{\varepsilon^2} \Omega^* S^*}, \quad A_5 = \frac{1.6 C_\mu \bar{\rho} \frac{k^2}{\varepsilon}}{\bar{\rho} \frac{k^4}{\varepsilon^3} \frac{7S^* S^* + \Omega^* \Omega^*}{4}}, \tag{25}$$

in which,

$$A_s = \sqrt{6} \cos \varphi, \quad \varphi = \frac{1}{3} \arccos(\sqrt{6} W^*), \quad W^* = \frac{S_{ij}^* S_{jk}^* S_{ki}^*}{(S^*)^3}, \tag{26}$$

$$U^* = \sqrt{(S^*)^2 + (\Omega^*)^2}, \quad S^* = \sqrt{S_{ij}^* S_{ij}^*}, \quad \Omega^* = \sqrt{\tilde{\Omega}_{ij} \tilde{\Omega}_{ij}}, \quad S_{ij}^* = \tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{kk} \tag{27}$$

The coefficient f is a function of the resolution control parameter (RCP) that is defined as a ratio of the time filter width Δ_T to a global integral time scale of the flow T : $RCP = \Delta_T / T$ and

$$f\left(\frac{\Delta_T}{T}\right) \approx 2\left(\frac{\Delta_T}{T}\right) - \left(\frac{\Delta_T}{T}\right)^2 \tag{28}$$

As it is discussed in Reference 7 that RCP represents the percentage of unresolved turbulent kinetic energy. Therefore, the value of RCP and the coefficient f are always between 0 and 1. Similarly, the nonlinear model for subscale scalar fluxes is formulated as (Ref. 16)

$$\Theta_i = -\vartheta_T \frac{\partial \bar{\rho} \tilde{\theta}}{\partial x_i} - \vartheta_T \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial \bar{\rho} \tilde{\theta}}{\partial x_j} \tag{29}$$

Where ϑ_T denotes the subscale turbulent diffusivity for the corresponding scalar quantity θ . It is often approximated by $\vartheta_T = \nu_T / \text{Pr}^\theta$, and Pr^θ represents the turbulent Prandtl number or Schmidt number depending on whether the scalar quantity $\tilde{\theta}$ is the energy $\tilde{\varepsilon}$ or the species $\tilde{\Phi}_m$. The subscale turbulent eddy viscosity is defined as $\nu_T = f \cdot C_\mu \cdot k^2 / \varepsilon$. The coefficients, c_1 and c_2 , are yet to be calibrated. In the current simulations they are set to be $c_1 = c_2 = -0.24$.

The subscale turbulent kinetic energy and its dissipation rate k , ε will be determined from the following model equations:

$$\frac{\partial}{\partial t} \bar{\rho} k + \frac{\partial}{\partial x_i} \bar{\rho} \tilde{u}_i k = \frac{\partial}{\partial x_i} \left[(\mu + \mu_T) \frac{\partial}{\partial x_i} k \right] - \tau_{ij} \tilde{S}_{ij} - \bar{\rho} \varepsilon \tag{30}$$

$$\frac{\partial}{\partial t} \bar{\rho} \varepsilon + \frac{\partial}{\partial x_i} \bar{\rho} \tilde{u}_i \varepsilon = \frac{\partial}{\partial x_i} \left[(\mu + \mu_T) \frac{\partial}{\partial x_i} \varepsilon \right] - C_{\varepsilon 1} \tau_{ij} \tilde{s}_{ij} \frac{\varepsilon}{k} - C_{\varepsilon 2} \frac{\bar{\rho} \varepsilon^2}{k} \quad (31)$$

where $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are the model coefficients. We have adopted the commonly used values of $C_{\varepsilon 1} = 1.45$ and $C_{\varepsilon 2} = 1.92$ in the present work while keeping in mind that here μ_T is a subscale turbulent eddy viscosity.

3.0 Basic Equation for Scalar DWFDF

In this Section, we will use the fine grained probability density function (FG-PDF) to define the density weighted time filtered fine grained probability density function (DWFDF), then explore the relationship between scalar DWFDF and time filtered turbulent scalar variables. This will provide the basis for establishing the transport equation for the scalar DWFDF.

3.1 Definition of Scalar DWFDF

3.1.1 Fine Grained Probability Density Function (FG-PDF) for Scalars $f'_\Phi(\psi; \mathbf{x}, t)$

According to Pope's definition (Ref. 1), the joint FG-PDF for turbulent velocity and scalars (i.e., compositions or species mass fractions, internal energy) can be written as

$$\begin{aligned} f'(V, \psi; \mathbf{x}, t) &\equiv \delta(\mathbf{U}(\mathbf{x}, t) - \mathbf{V}) \delta(\Phi(\mathbf{x}, t) - \psi) \\ &\equiv \prod_{i=1}^3 \delta(U_i(\mathbf{x}, t) - V_i) \prod_{m=1}^{M+1} \delta(\Phi_m(\mathbf{x}, t) - \psi_m) \end{aligned} \quad (32)$$

Its marginal FG-PDF for scalars is

$$f'_\Phi(\psi; \mathbf{x}, t) \equiv \delta(\Phi(\mathbf{x}, t) - \psi) \equiv \prod_{m=1}^{M+1} \delta(\Phi_m(\mathbf{x}, t) - \psi_m) \quad (33)$$

where δ denotes the delta function, $\mathbf{U}(\mathbf{x}, t)$ is the turbulent (random) velocity vector (U_1, U_2, U_3), $\Phi(\mathbf{x}, t)$ is the turbulent (random) scalar array ($\Phi_1, \Phi_2, \dots, \Phi_M, \Phi_{M+1}$), for example, M species mass fractions and one internal energy $\Phi_{M+1} = e$; the $\mathbf{x}, t$ denote the physical space variable (x_1, x_2, x_3) and the time t , $\mathbf{V} \equiv (V_1, V_2, V_3)$ and $\psi \equiv (\psi_1, \psi_2, \dots, \psi_M, \psi_{M+1})$ are the sample space variables for $\mathbf{U}(\mathbf{x}, t)$ and $\Phi(\mathbf{x}, t)$, respectively.

3.1.2 Scalar DWFDF $F_\Phi(\psi; \mathbf{x}, t)$

We define the following density weighted time filtered fine-grained probability density function for scalars as

$$\begin{aligned} F_\Phi(\psi; \mathbf{x}, t) &\equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') f'_\Phi(\psi; \mathbf{x}, t') G(t - t') dt' \\ &= \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') \delta(\Phi(\mathbf{x}, t') - \psi) G(t - t') dt' \end{aligned} \quad (34)$$

Obviously, the scalar DWFDF, $F_\Phi(\psi; \mathbf{x}, t)$, is still a random quantity. And it satisfies the following “normalization” property:

$$\int_{-\infty}^{\infty} F_{\Phi}(\boldsymbol{\psi}; \mathbf{x}, t) d\boldsymbol{\psi} = \int_{-\infty}^{\infty} \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') \delta(\boldsymbol{\Phi} - \boldsymbol{\psi}) G(t - t') dt' d\boldsymbol{\psi} = \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') G(t - t') dt' = \bar{\rho} \quad (35)$$

Note that here $\int_{-\infty}^{\infty}$ means that the integration is over the entire domain of the sample space $\boldsymbol{\psi}$.

3.1.3 Relationship Between Scalar DWFDF and Large Scale Turbulent Scalar Variables

With the definition of scalar DWFDF described in Equation (34), we can exactly deduce the density weighted time filtered scalar turbulent variables that are defined in Equations (1) and (4). For example,

$$\begin{aligned} \int_{-\infty}^{+\infty} \boldsymbol{\psi} F_{\Phi}(\boldsymbol{\psi}; \mathbf{x}, t) d\boldsymbol{\psi} &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \boldsymbol{\psi} \rho(\mathbf{x}, t') \delta(\boldsymbol{\Phi}(\mathbf{x}, t') - \boldsymbol{\psi}) G(t - t') dt' d\boldsymbol{\psi} \\ &= \int_{-\infty}^{+\infty} \boldsymbol{\Phi}(\mathbf{x}, t') \rho(\mathbf{x}, t') G(t - t') dt' \\ &= \overline{\rho \boldsymbol{\Phi}} = \bar{\rho}(\mathbf{x}, t) \widetilde{\boldsymbol{\Phi}}(\mathbf{x}, t) \end{aligned} \quad (36)$$

Equation (36) indicates that the left hand side is an operation $\langle \boldsymbol{\Phi} \rangle$ that defines the density weighed time filtered turbulent variable $\overline{\rho \boldsymbol{\Phi}}$:

$$\langle \boldsymbol{\Phi} \rangle \equiv \int_{-\infty}^{+\infty} \boldsymbol{\psi} F_{\Phi}(\boldsymbol{\psi}; \mathbf{x}, t) d\boldsymbol{\psi} = \bar{\rho}(\mathbf{x}, t) \widetilde{\boldsymbol{\Phi}}(\mathbf{x}, t) \quad (37)$$

For a function $W(\boldsymbol{\Phi}(\mathbf{x}, t))$, it is easy to verify that

$$\langle W(\boldsymbol{\Phi}) \rangle = \int_{-\infty}^{+\infty} W(\boldsymbol{\psi}) F_{\Phi}(\boldsymbol{\psi}; \mathbf{x}, t) d\boldsymbol{\psi} = \bar{\rho}(\mathbf{x}, t) \widetilde{W}(\boldsymbol{\Phi}(\mathbf{x}, t)) \quad (38)$$

Furthermore, we may consider the derivatives $\nabla \boldsymbol{\Phi}$ as a new random quantity and legitimately write

$$\langle \nabla \boldsymbol{\Phi} \rangle = \bar{\rho} \widetilde{\nabla \boldsymbol{\Phi}} \quad (39)$$

However, because of the variable density, the “operation” $\langle \rangle$ does not have the differential commute property, i.e.,

$$\langle \nabla \boldsymbol{\Phi} \rangle \neq \nabla \langle \boldsymbol{\Phi} \rangle \quad (40)$$

because $\bar{\rho} \widetilde{\nabla \boldsymbol{\Phi}} \neq \nabla(\bar{\rho} \widetilde{\boldsymbol{\Phi}})$.

We can also write the density weighted time filtered $\langle U_j \Phi_i \rangle$ for the joint velocity and scalar variables as

$$\langle U_j \Phi_i \rangle = \int_{-\infty}^{+\infty} V_j \psi_i F_{U, \Phi}(V, \boldsymbol{\psi}; \mathbf{x}, t) dV d\boldsymbol{\psi} = \bar{\rho}(\mathbf{x}, t) \widetilde{U_j \Phi_i}(\mathbf{x}, t) \quad (41)$$

where, $F_{U, \Phi}(V, \boldsymbol{\psi}; \mathbf{x}, t)$ is the joint DWFDF defined as

$$F_{U, \Phi}(V, \boldsymbol{\psi}; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') \delta(U(\mathbf{x}, t') - V) \delta(\boldsymbol{\Phi}(\mathbf{x}, t') - \boldsymbol{\psi}) G(t - t') dt' \quad (42)$$

which also satisfies the “normalization” property:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_{U, \Phi}(V, \boldsymbol{\psi}; \mathbf{x}, t) dV d\boldsymbol{\psi} = \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') G(t - t') dt' = \bar{\rho} \quad (43)$$

3.1.4 Joint DWFDF, $F_{U,\Phi}(V, \psi; \mathbf{x}, t)$ and Its Conditional DWFDF $F_{U|\Phi}(V|\psi; \mathbf{x}, t)$

From Equation(42), we may follow Reference 1 to define a “conditional” DWFDF on the condition $\Phi = \psi$ as

$$F_{U|\Phi}(V|\psi; \mathbf{x}, t) \equiv \frac{F_{U,\Phi}(V, \psi; \mathbf{x}, t)}{F_{\Phi}(\psi; \mathbf{x}, t)} \quad (44)$$

and the “conditional filtering” (or conditional ‘mean’) as

$$\begin{aligned} \langle U(\mathbf{x}, t) | \psi \rangle &\equiv \int_{-\infty}^{+\infty} V F_{U|\Phi}(V|\psi; \mathbf{x}, t) dV = \frac{1}{F_{\Phi}(\psi; \mathbf{x}, t)} \int_{-\infty}^{+\infty} V F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV \\ &= \frac{1}{F_{\Phi}} \int_{-\infty}^{+\infty} V \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') \delta(U(\mathbf{x}, t') - V) \delta(\Phi(\mathbf{x}, t') - \psi) G(t - t') dt' dV \\ &= \frac{1}{F_{\Phi}} \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') U(\mathbf{x}, t') \delta(\Phi(\mathbf{x}, t') - \psi) G(t - t') dt' \end{aligned} \quad (45)$$

Then we have

$$\int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') U(\mathbf{x}, t') f'_{\Phi}(\psi; \mathbf{x}, t') G(t - t') dt' = \int_{-\infty}^{+\infty} V F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV = F_{\Phi} \cdot \langle U(\mathbf{x}, t) | \psi \rangle \quad (46)$$

And the “complete” filtering should be

$$\begin{aligned} \int_{-\infty}^{+\infty} (F_{\Phi} \cdot \langle U(\mathbf{x}, t) | \psi \rangle) d\psi &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} V F_{U,\Phi}(V, \psi; \mathbf{x}, t) dV d\psi \\ &= \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') U(\mathbf{x}, t') G(t - t') dt' \\ &= \bar{\rho}(\mathbf{x}, t) \tilde{U}(\mathbf{x}, t) \end{aligned} \quad (47)$$

Equation (46) can be extended to any other turbulent quantities, for example, $\nabla \Phi$, $S_i(\Phi)$:

$$\begin{aligned} \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') \nabla \Phi(\mathbf{x}, t') f'_{\Phi}(\psi; \mathbf{x}, t') G(t - t') dt' &= F_{\Phi} \cdot \langle \nabla \Phi | \psi \rangle \\ \int_{-\infty}^{+\infty} \rho(\mathbf{x}, t') S_i(\Phi(\mathbf{x}, t')) f'_{\Phi}(\psi; \mathbf{x}, t') G(t - t') dt' &= F_{\Phi} \cdot \langle S_i(\Phi) | \psi \rangle = F_{\Phi} \cdot S_i(\psi) \end{aligned} \quad (48)$$

Where $\nabla \Phi$ is viewed as a new random variable in addition to Φ .

3.2 Transport Equation for Scalar DWFDF $F_{\Phi}(\psi; \mathbf{x}, t)$

We can now derive the transport equation for scalar DWFDF from Equations (18), (19) as follows: first, we write the terms on the left hand side of Equation (19) as

$$\frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial t} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi_m F_{\Phi} d\psi = \int_{-\infty}^{\infty} \psi_m \frac{\partial F_{\Phi}}{\partial t} d\psi \quad (49)$$

$$\frac{\partial \overline{\rho U_i \Phi_m}}{\partial x_i} = \frac{\partial}{\partial x_i} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} V_i \psi_m F_{U,\Phi} dV d\psi = \begin{cases} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_m \left(V_i \frac{\partial}{\partial x_i} F_{U,\Phi} \right) dV d\psi \\ \text{or} \\ \int_{-\infty}^{\infty} \psi_m \left(\frac{\partial}{\partial x_i} (F_\Phi \cdot \langle U_i | \psi \rangle_L) \right) d\psi \end{cases} \quad (50)$$

Then, the terms on the right hand side of (19) can be written as

$$\frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial \overline{\rho \Phi_m}}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial}{\partial x_i} \int_{-\infty}^{\infty} \psi_m F_\Phi d\psi \right) = \int_{-\infty}^{\infty} \psi_m \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_\Phi}{\partial x_i} \right) d\psi \quad (51)$$

$$\overline{\rho \tilde{S}_m} = \int_{-\infty}^{\infty} S_m(\psi) F_\Phi d\psi = - \int_{-\infty}^{\infty} \psi_m \frac{\partial (S_k F_\Phi)}{\partial \psi_k} d\psi \quad (52)$$

Where in Equation (52) we have applied the integration by parts and the following zero integration:

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial \psi} [A(\psi) \cdot F_\Phi] d\psi = 0, \quad \text{if a finite value of filtering } \langle A \rangle \text{ exists.} \quad (53)$$

Collecting all the integrand terms, and let the sum be zero (we refer this as the conservation condition, which is in general a sufficient but may not be necessary condition, Ref. 17), we obtain

$$\frac{\partial F_\Phi}{\partial t} + \frac{\partial (F_\Phi \cdot \langle U_i | \psi \rangle)}{\partial x_i} = \left\{ \frac{\partial}{\partial x_i} \left(\Gamma^{(m)} \frac{\partial F_\Phi}{\partial x_i} \right) - \frac{\partial}{\partial \psi_k} [F_\Phi \cdot S_k(\psi)] \right\}, \quad k = 1, 2, \dots, M+1 \quad (54)$$

This equation also includes the equation of internal energy when $S_{M+1}(\psi) = 0$ and other source terms in Equation (18) are neglected. Unlike the case of the joint DWFDF $F_{U,\Phi}$, for the marginal F_Φ , the convection term is not closed because of the conditional filtering $\langle U_i | \psi \rangle$. Then, this critically important term,

corresponding to $\overline{\rho \tilde{U}_i \Phi_m}$ in Equation (19), must be carefully modeled while the less important molecular diffusion term naturally remains in the closed form. In addition, we noticed that the equally important chemistry source term $\overline{\rho \tilde{S}_m(\Phi)}$ in Equation (19), which involves complex processes of turbulence-chemistry interaction, is closed in the scalar DWFDF equation, i.e., no need of modeling. This direct calculation of turbulence-chemistry interaction is one of the unique features of the PDF methodology.

3.3 Nonlinear Model for Subscale Scalar Fluxes

The convection term in Equation (54) contains the term $F_\Phi \cdot \langle U_i | \psi \rangle$, which must be modeled. We may start from a nonlinear model, Equation (29), for the term $\overline{\rho \tilde{U}_i \Phi_m}$:

$$\overline{\rho \tilde{U}_i \Phi_m} = \overline{\rho \tilde{U}_i \tilde{\Phi}_m} - \Gamma_T^{(m)} \frac{\partial \overline{\rho \tilde{\Phi}_m}}{\partial x_i} - \Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial \overline{\rho \tilde{\Phi}_m}}{\partial x_j} \quad (55)$$

This will lead to the following model by directly applying Equations (37) and (46):

$$F_\Phi \cdot \langle U_i | \Psi \rangle = \tilde{U}_i F_\Phi - \left[\Gamma_T^{(m)} \frac{\partial F_\Phi}{\partial x_i} \right] + \frac{\partial}{\partial \psi_k} \left[\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \psi_k \frac{\partial F_\Phi}{\partial x_j} \right] \quad (56)$$

3.4 Summary

With the model given by Equation (56), the scalar DWDFD equation for $F_\Phi(\Psi; \mathbf{x}, t)$ can be written as

$$\begin{aligned} \frac{\partial F_\Phi}{\partial t} + \frac{\partial (\tilde{U}_i F_\Phi)}{\partial x_i} = & \left\{ \frac{\partial}{\partial x_i} \left(\left(\Gamma^{(m)} + \Gamma_T^{(m)} \right) \frac{\partial F_\Phi}{\partial x_i} \right) \right\} - \frac{\partial}{\partial \psi_k} (F_\Phi \cdot S_k(\Psi)) \\ & - \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left(\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial F_\Phi}{\partial x_j} \right) \right\}, \quad k = 1, 2, \dots, M+1 \end{aligned} \quad (57)$$

It can be verified that the scalar DWDFD Equation (57) can exactly deduce the time filtered equation (19).

However, the model described by this equation is by no means unique. In addition, the variables ($\tilde{U}_i$, $\tilde{S}_{ij}$ and $\tilde{\Omega}_{ij}$) are considered to be available during the solution procedure of the scalar DWDFD equation.

Furthermore, in order to apply the available stochastic solution procedure built in the NCC code, we further simplify the model term in Equation (57) as follows:

$$- \frac{\partial}{\partial \psi_k} \left\{ \psi_k \frac{\partial}{\partial x_i} \left(\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial F_\Phi}{\partial x_j} \right) \right\} = \frac{\partial}{\partial \psi_k} \left(\psi_k \frac{1}{\tau} F_\Phi \right) \quad (58)$$

where

$$\frac{1}{\tau} \equiv - \frac{1}{F_\Phi} \frac{\partial}{\partial x_i} \left(\Gamma_T^{(m)} \frac{k}{\varepsilon} (c_1 \tilde{S}_{ij} + c_2 \tilde{\Omega}_{ij}) \frac{\partial F_\Phi}{\partial x_j} \right) \approx \sqrt{\tilde{S}_{ij} \tilde{S}_{ij} + \tilde{\Omega}_{ij} \tilde{\Omega}_{ij}} \quad (59)$$

Equation (59) is a crude approximation based on the dimensional argument for a time scale, which is responsible for the diffusion of scalar DWDFD in the sample variable space ψ_k . We chose this time scale to be related to the rate of strain and rotation instead of its complex formulation. In order to prevent this time scale from being non-physically small during the simulation, we require that

$$\tau \geq \sqrt{(\nu + \nu_T) / \varepsilon} \quad (60)$$

because the right hand side of (60) represents the smallest time scale of the simulated flow field.

4.0 Numerical Simulations of Single Element LDI Injector

The lean direct injection (LDI) injector is a liquid fuel injector developed to reduce aircraft emissions. Stable combustion is essentially completed within a short distance through rapid fuel and air mixing. This design also allows for many small fuel injectors integrated into modules facilitating different fuel staging strategies, such as the one shown in Figure 1. So far, experimental observations have not fully clarified the dynamics of the mixing and combustion processes occurring in these injectors, and numerical studies need to be conducted to achieve a better understanding of the underlying physics of the LDI injector. Figure 2 shows the air swirler and the convergent-divergent nozzle of the single element injector. Figure 3 depicts the single element LDI combustor geometry and its computational domain. Five probes are dispatched along the centerline (Figure 4) to monitor the evolution of turbulent variables during the simulations. The numerical grid is formed using hexahedral elements and the total number of elements is about 862,000, which is a relatively coarse grid used in a previous RANS simulation (Ref.18).

In this study, the liquid fuel is Jet-A, and C12H23 is adopted as its surrogate, the fuel is injected at the throat of the nozzle, mixing with the swirling air that comes from the air swirlers which consists of six helical, axial vanes with downstream vane angles of 60°. A prescribed droplet-size distribution spray model is used.

In this section, we present the VLES results of TFNS approach with and without invoking Eulerian scalar DWDFD method. We started both simulations with a same initial flow field that was created by earlier simulations from URANS to TFNS at the end of time step of 93,000. In the pure TFNS simulations, the chemistry-turbulence interaction is modeled with a “laminar chemistry” formulation, in which the generation rate of compositions is determined by the “known” filtered turbulent variables. This simulation has been carried out up to 185,000 time steps with a time step $dt = 1 \times 10^{-6}$. In the TFNS simulations with invoking an Eulerian scalar DWDFD method, the compositions and internal energy will be determined by the scalar DWDFD equation while the flow field is still determined by the continuity and momentum equations of the filtered Navier-Stokes equations. Since the production rate of composition (chemistry-turbulence interaction) is in a closed form in the scalar DWDFD equation, it can be directly calculated without modeling. This simulation is carried out up to 198,000 time steps with the same size of time step. The stochastic numerical procedures for solving Eulerian scalar DWDFD equation and fuel spray equation are described in Reference 4 and adopted in the present simulations.

Figure 5 shows the general pictures of simulated spray reacting flow in a single element LDI injector by both methods. Most of the results will be presented side by side for comparisons. The main results are presented in terms of : 1) the convergence history of time accurate simulations, which reflects numerical



Figure 1.—Nine element LDI module.

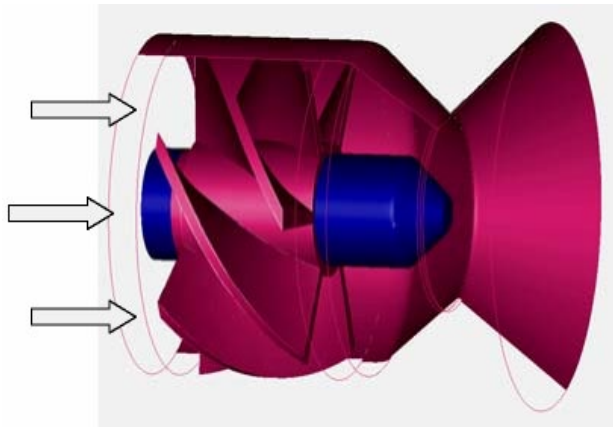


Figure 2.—Single element LDI injector.

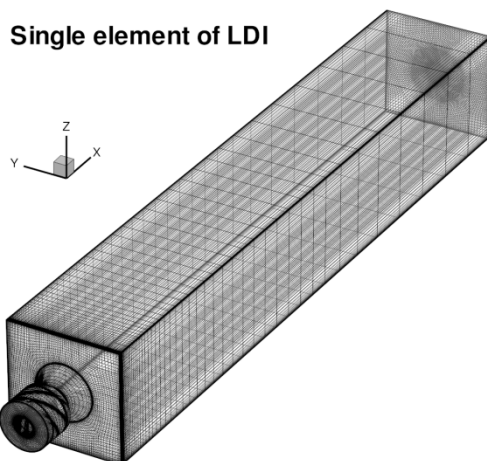


Figure 3.—Computational domain and grid spacing.

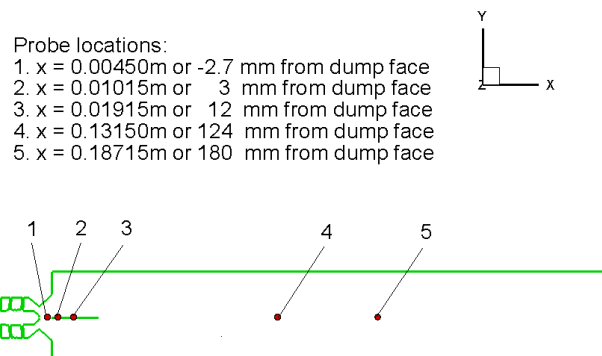


Figure 4.—Probes located along centerline.

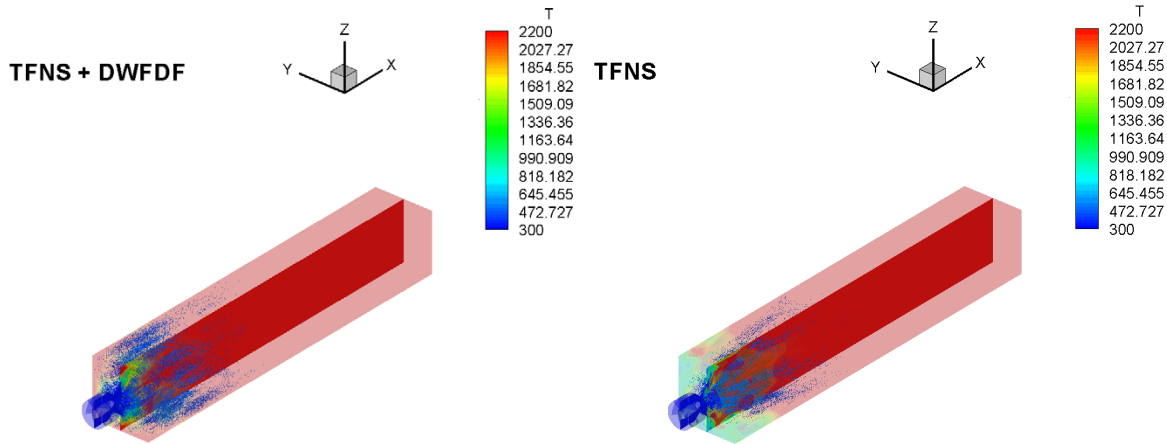


Figure 5.—Global pictures of spray reacting flow simulated with and without scalar DWFDF method.

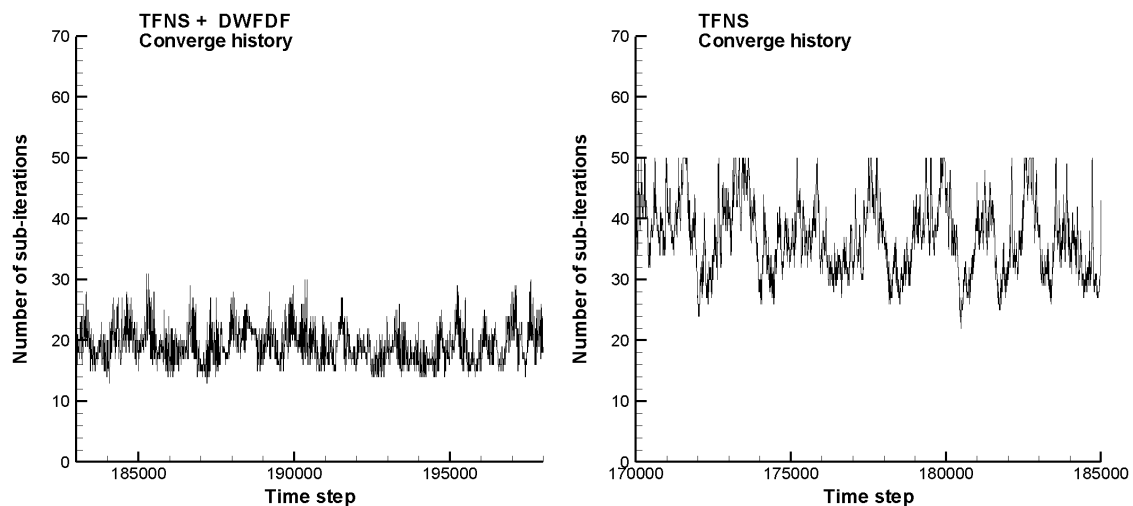


Figure 6.—Convergence histories of time accurate simulations.

performance, 2) the variations of velocity components and temperature versus the time step at five probes along the centerline (see Figure 4), which indicate the development of the simulated reacting flow, 3) the centerline distributions of mean (i.e., time averaged) temperature and mean axial velocity, 4) the mean temperature and mean velocity profiles along Z (crossing) axis at several downstream locations, 5) the center recirculation zone visualized by an iso-surface of zero mean axial velocity and the contour plots of various mean and instantaneous turbulent quantities in the X-Z center plane. These profiles, iso-surface and contour plots will provide the information about flow and flame structures of the simulated spray reacting flow. Some available experimental data (Ref. 19) are also plotted for comparisons with the numerical simulations.

4.1 Convergence History

Figure 6 shows the time history of the number of subiterations incurred in time accurate simulations with and without invoking the Eulerian scalar DWFDF method over the last 15,000 time steps. It is interesting to see that the simulation with the Eulerian scalar DWFDF method converges faster than the simulation without invoking scalar DWFDF method. For each time step, the former converges after about 20 subiterations, but the later often needs much more subiterations to converge. Comparing the wall time of computing, the simulation with DWFDF is about 34 hr with 256 processors for the 15,000 time steps; however, the simulation without DWFDF needs over 40 hr to finish 15,000 time steps of calculations.

4.2 Time Variation of Instantaneous Variables at Centerline Probes

Time history of temperature and velocity components at five downstream locations are recorded during the simulations (see Figure 7), it can be seen that at the first three locations the flow appears to be strongly fluctuated and fully developed turbulence (see both the instantaneous temperature T and axial velocity u).

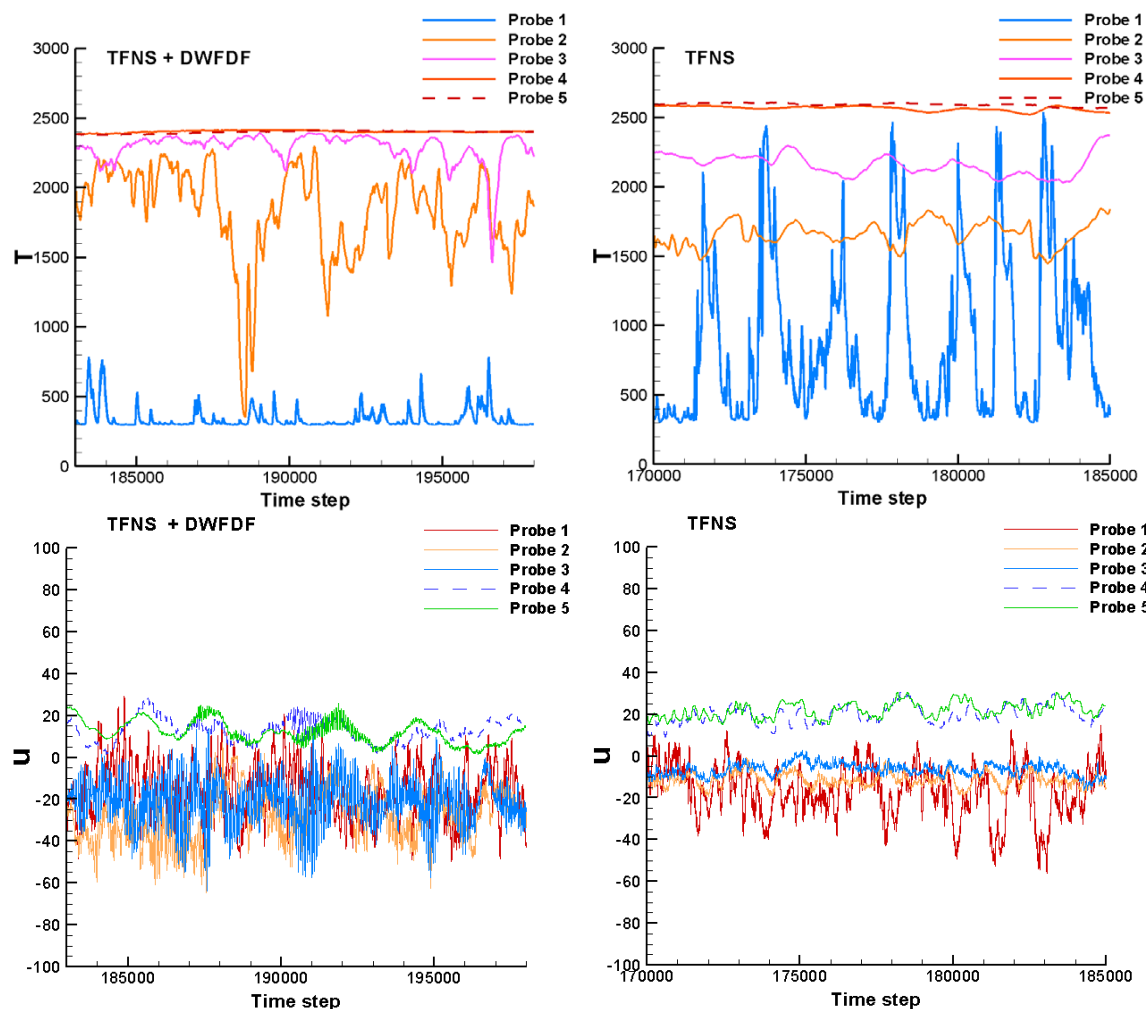


Figure 7.—Time history of temperature T and velocity components u , v and w at 5 probes.

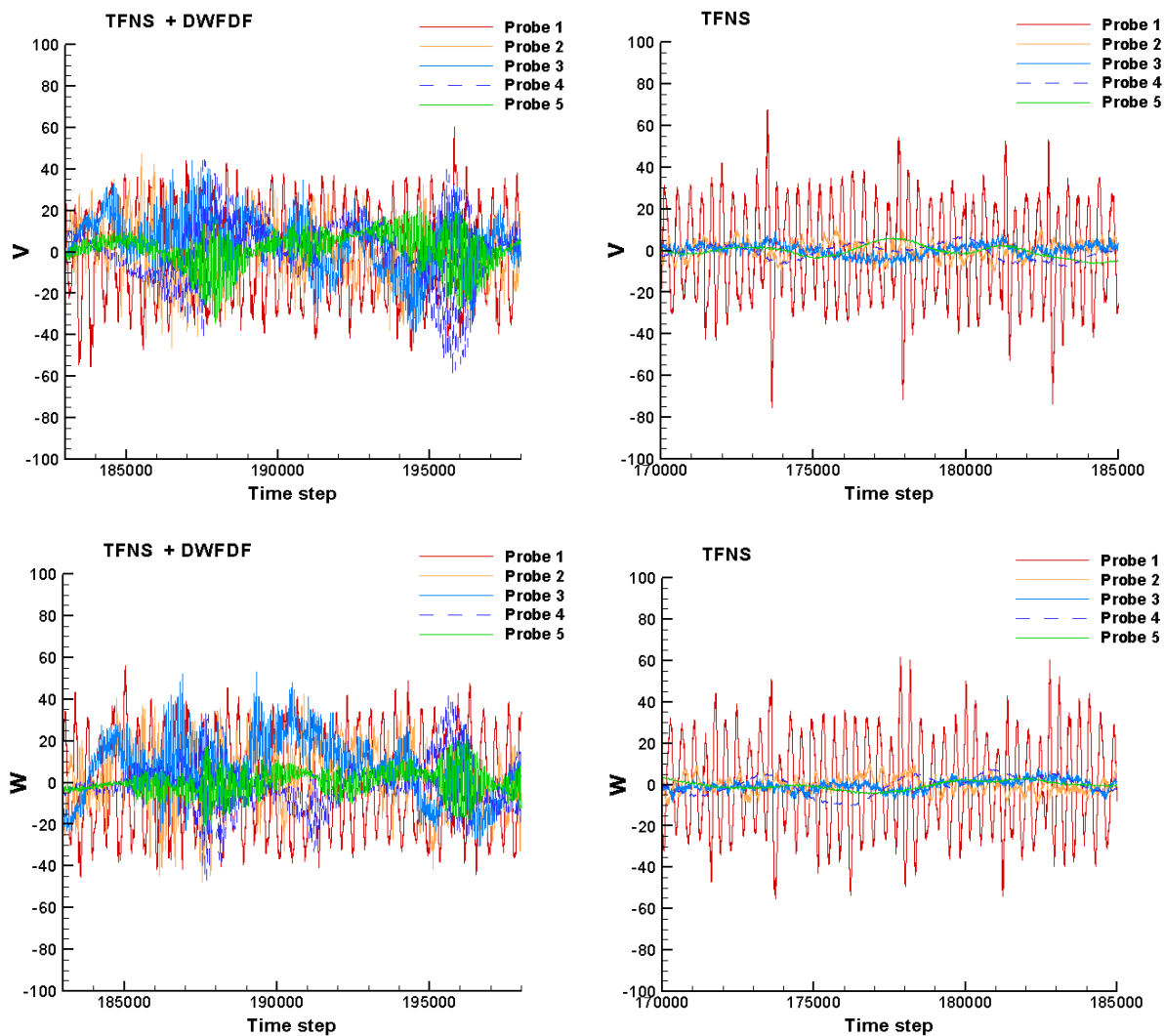


Figure 7.—Concluded.

4.3 Centerline Distributions of Mean Axial Velocity and Temperature

Centerline distributions of mean axial velocity and temperature are shown in Figure 8 and Figure 9. The effect of scalar DWFDF equation on the simulation is noticeable and positive.

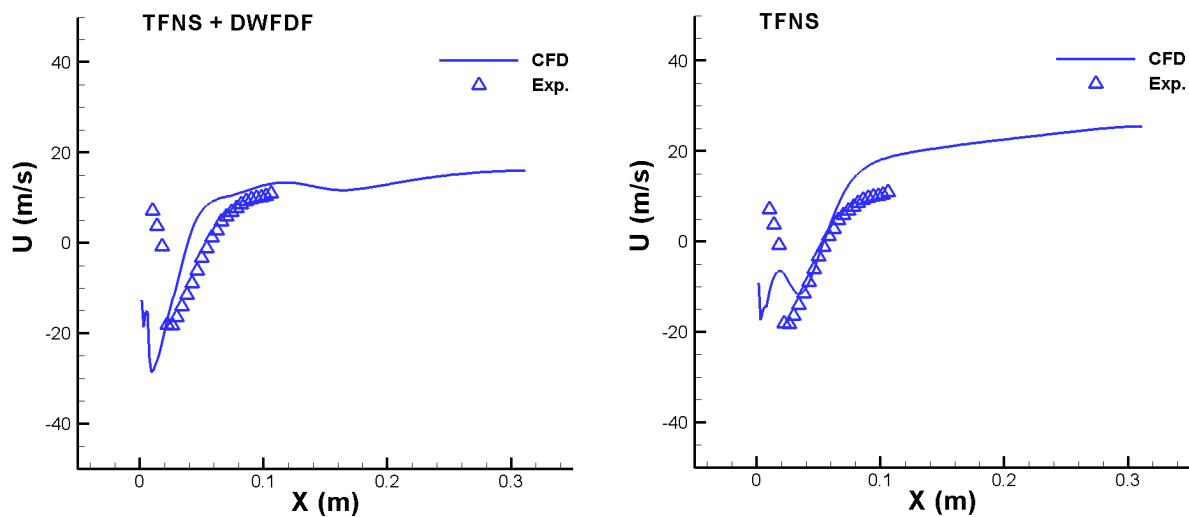


Figure 8.—Centerline distribution of mean axial velocity U .

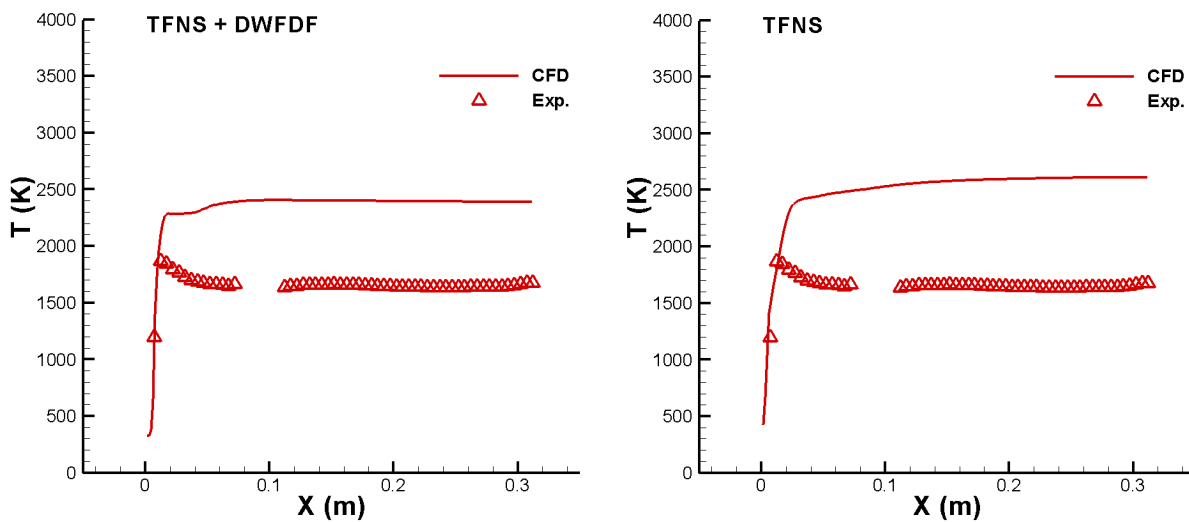


Figure 9.—Centerline distribution of mean temperature T .

4.4 Mean Temperature and Velocity Profiles Along Z Axis at Downstream Locations

Mean temperature profiles at downstream locations at $x = 5, 10, 20, 50, 110$ and 200 mm are compared and shown in Figure 10. These comparisons have revealed a positive effect of the DWFDF equation on the prediction of temperature. However, the effect of DWFDF equation on the velocity field, shown in Figure 11 and Figure 12, is mixed.

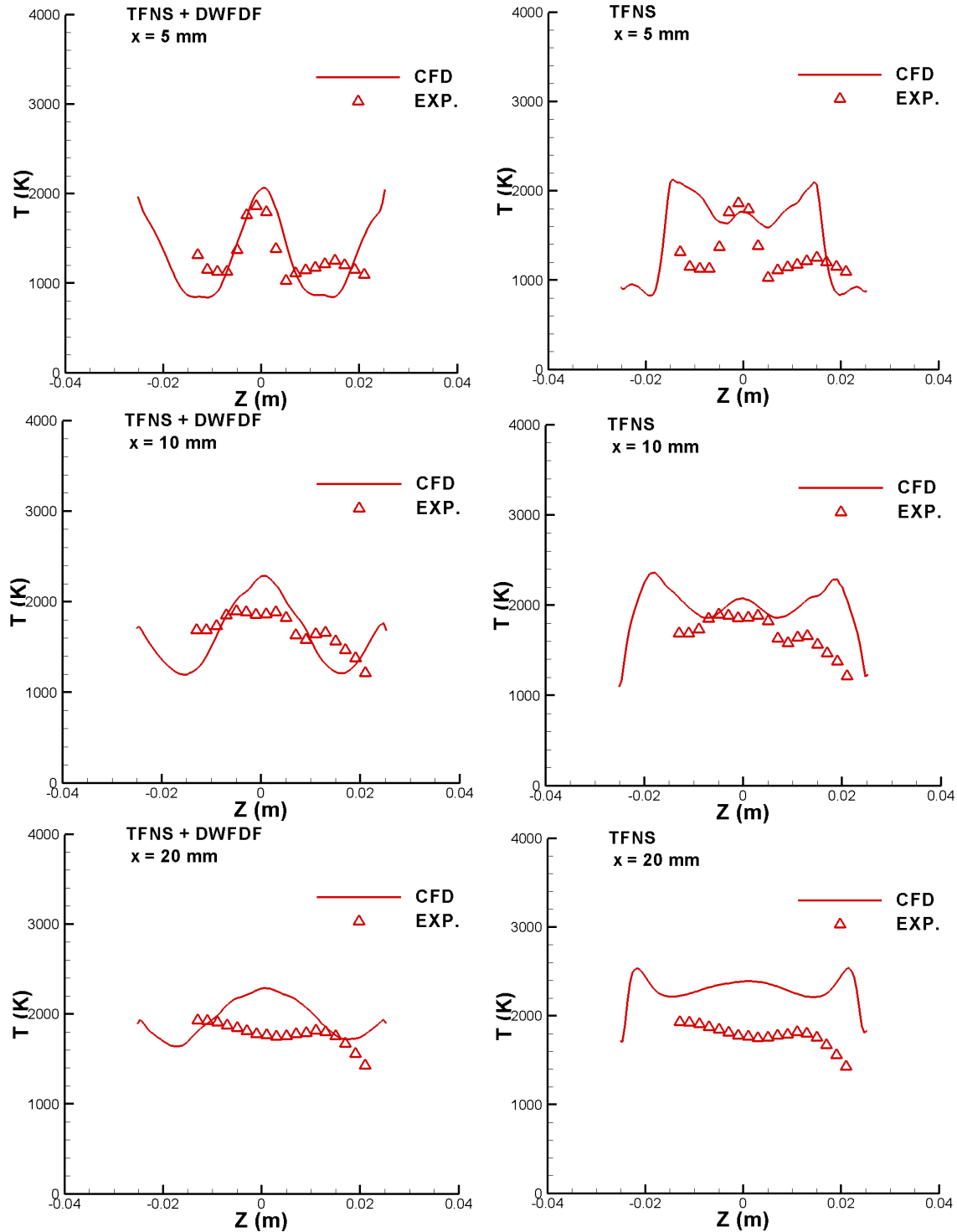


Figure 10.—Comparison of temperature distribution along Z axis at downstream locations.

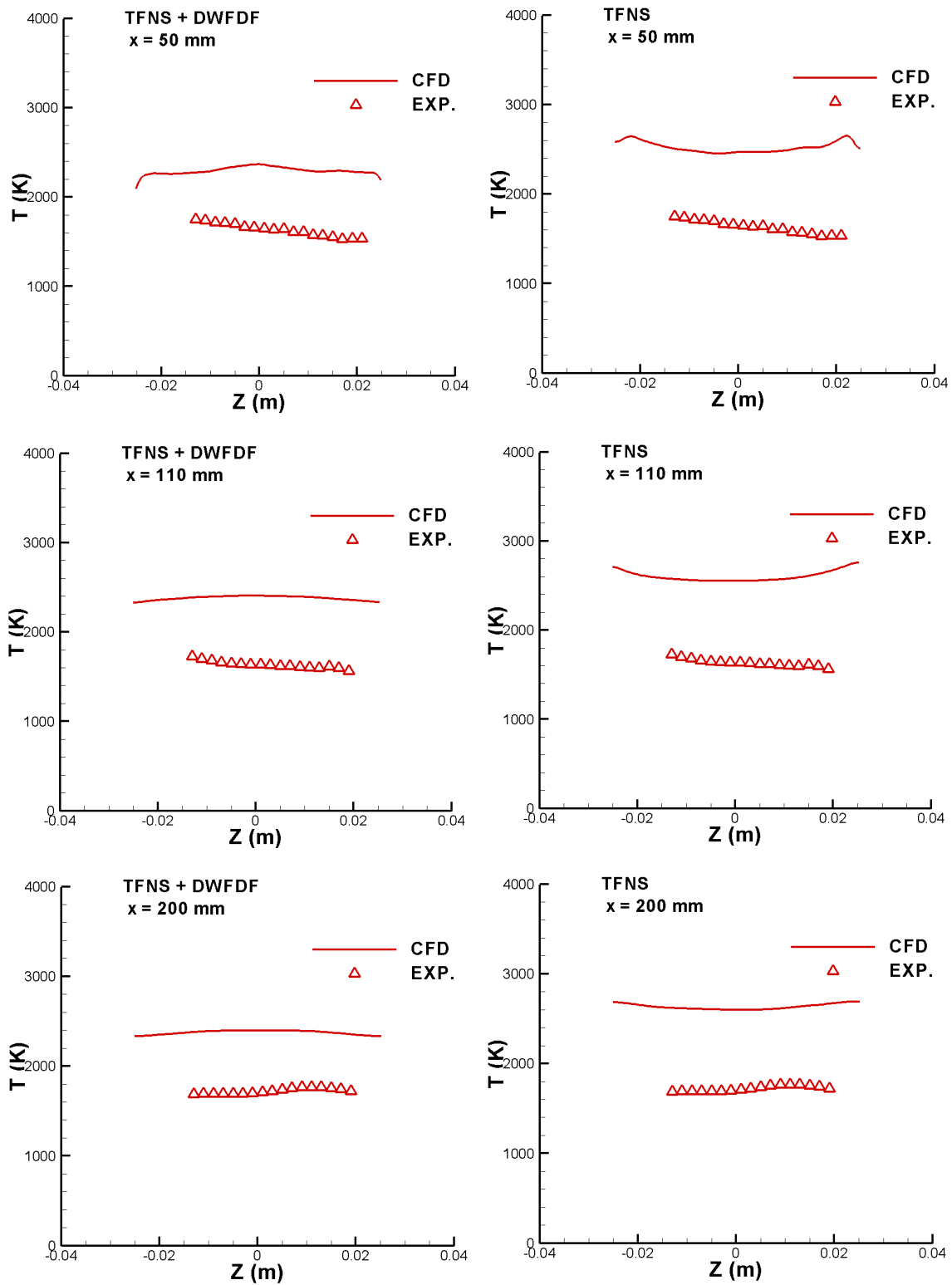


Figure 10.—Concluded.

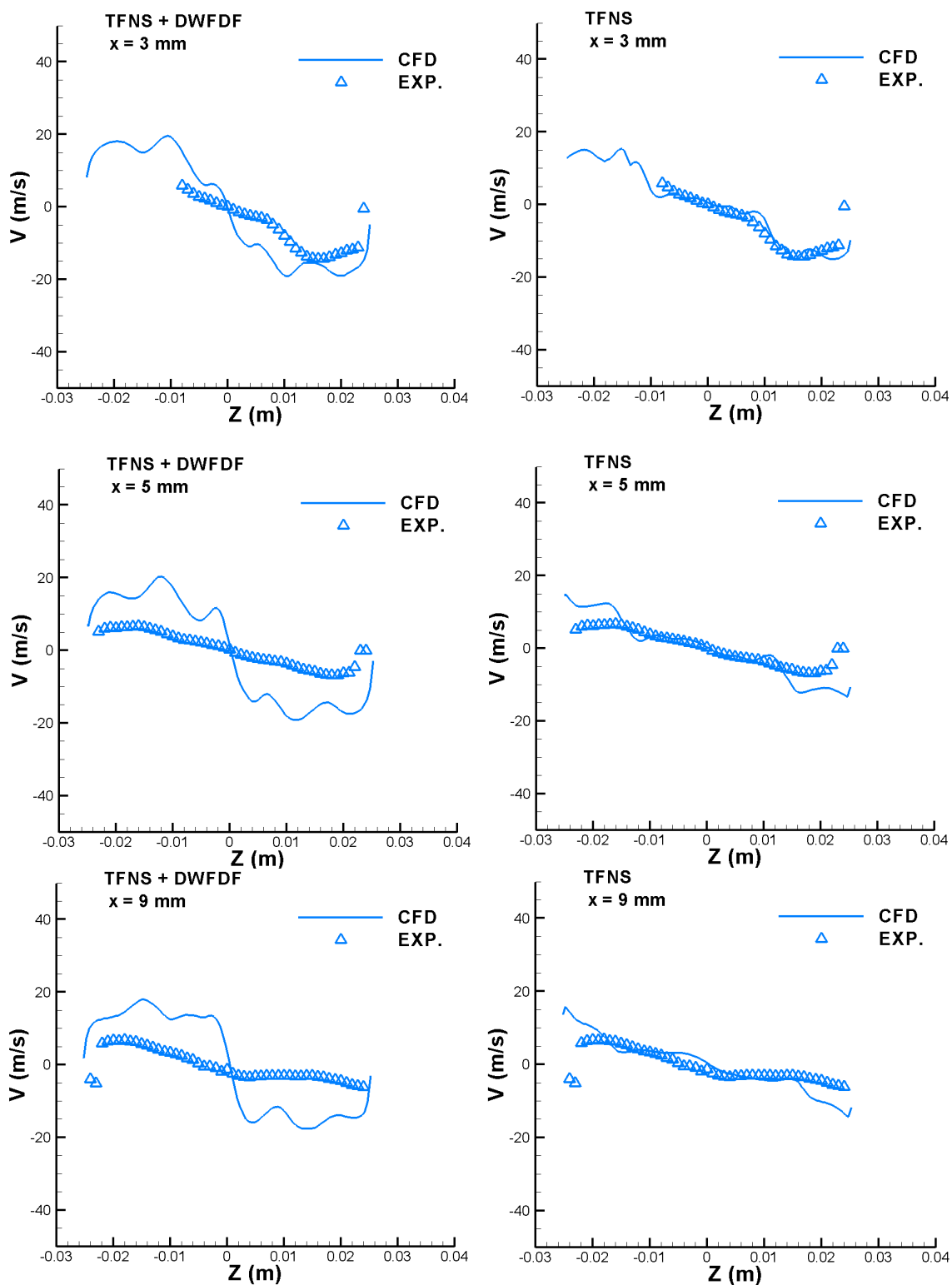


Figure 11.—Comparison of velocity component V along Z axis at downstream locations.

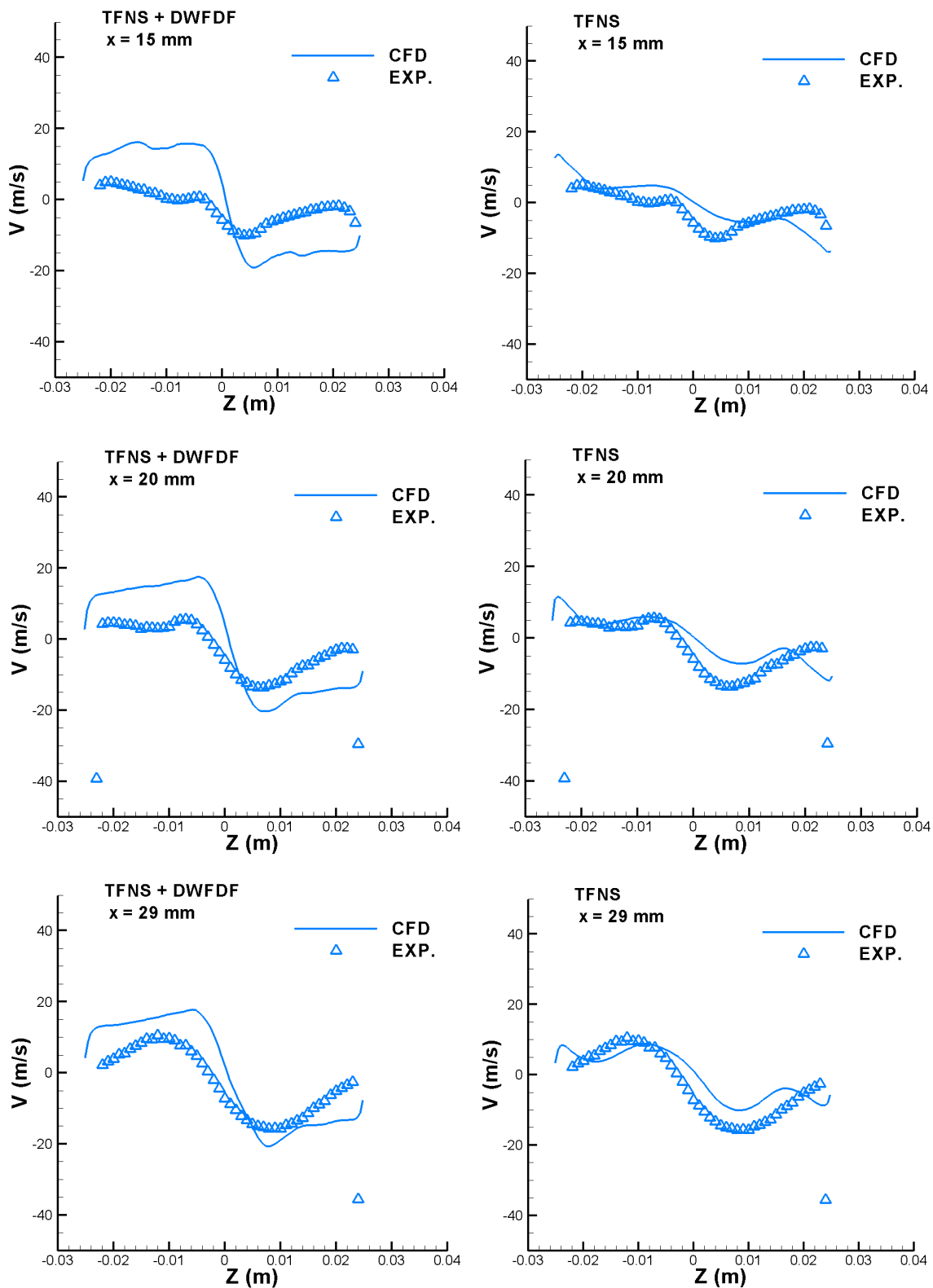


Figure 11.—Continued.

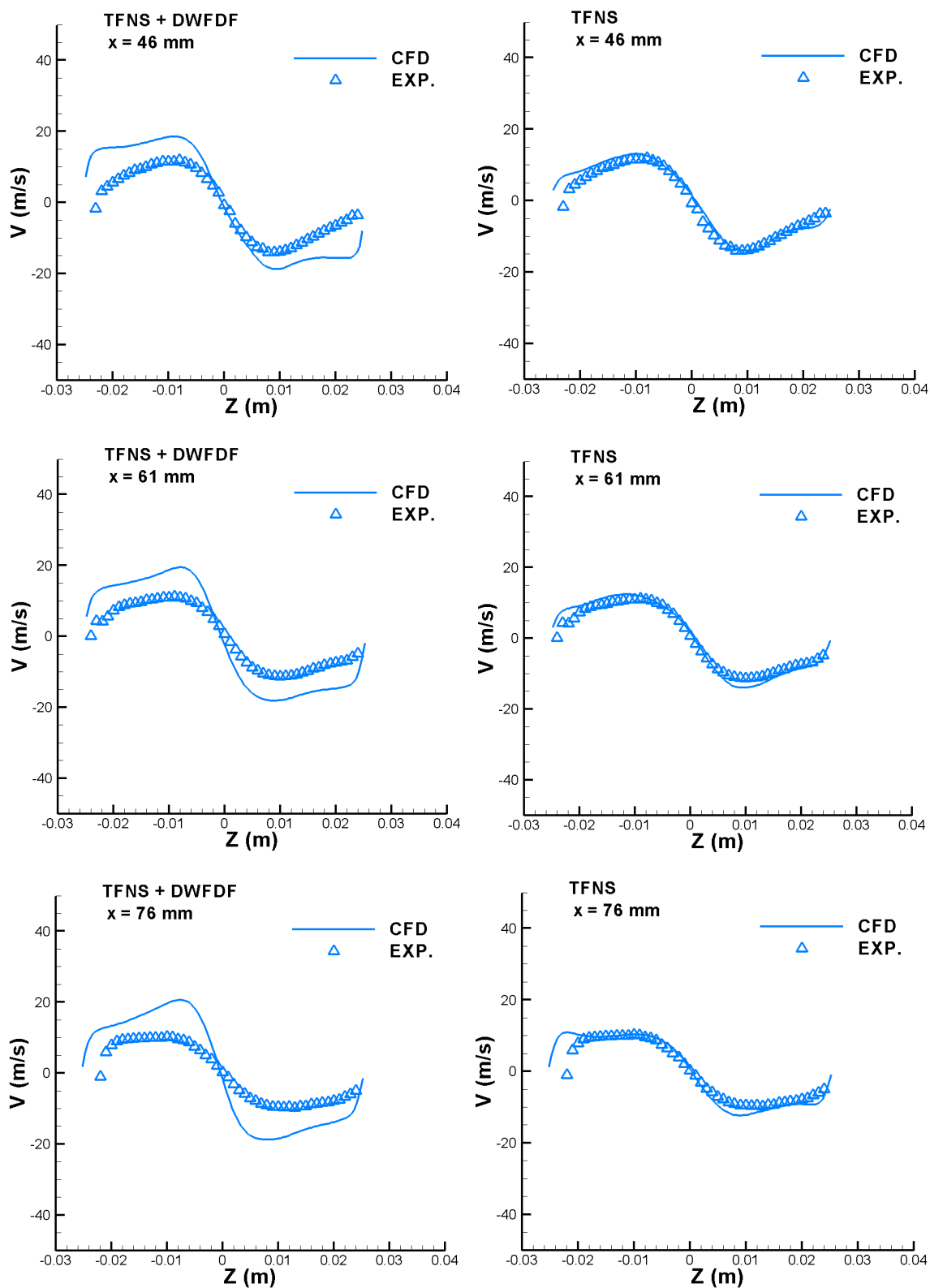


Figure 11.—Continued.

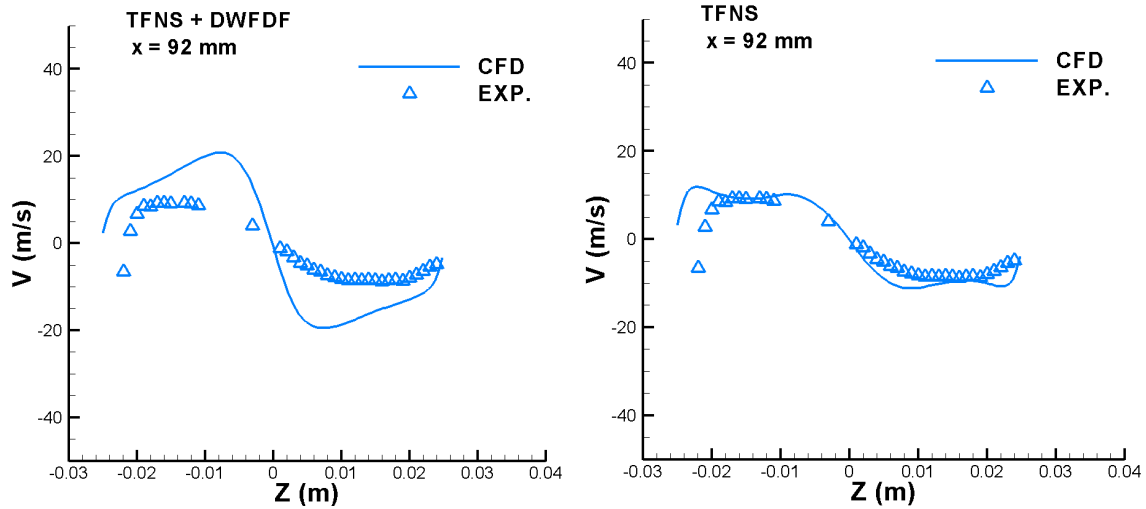


Figure 11.—Concluded.

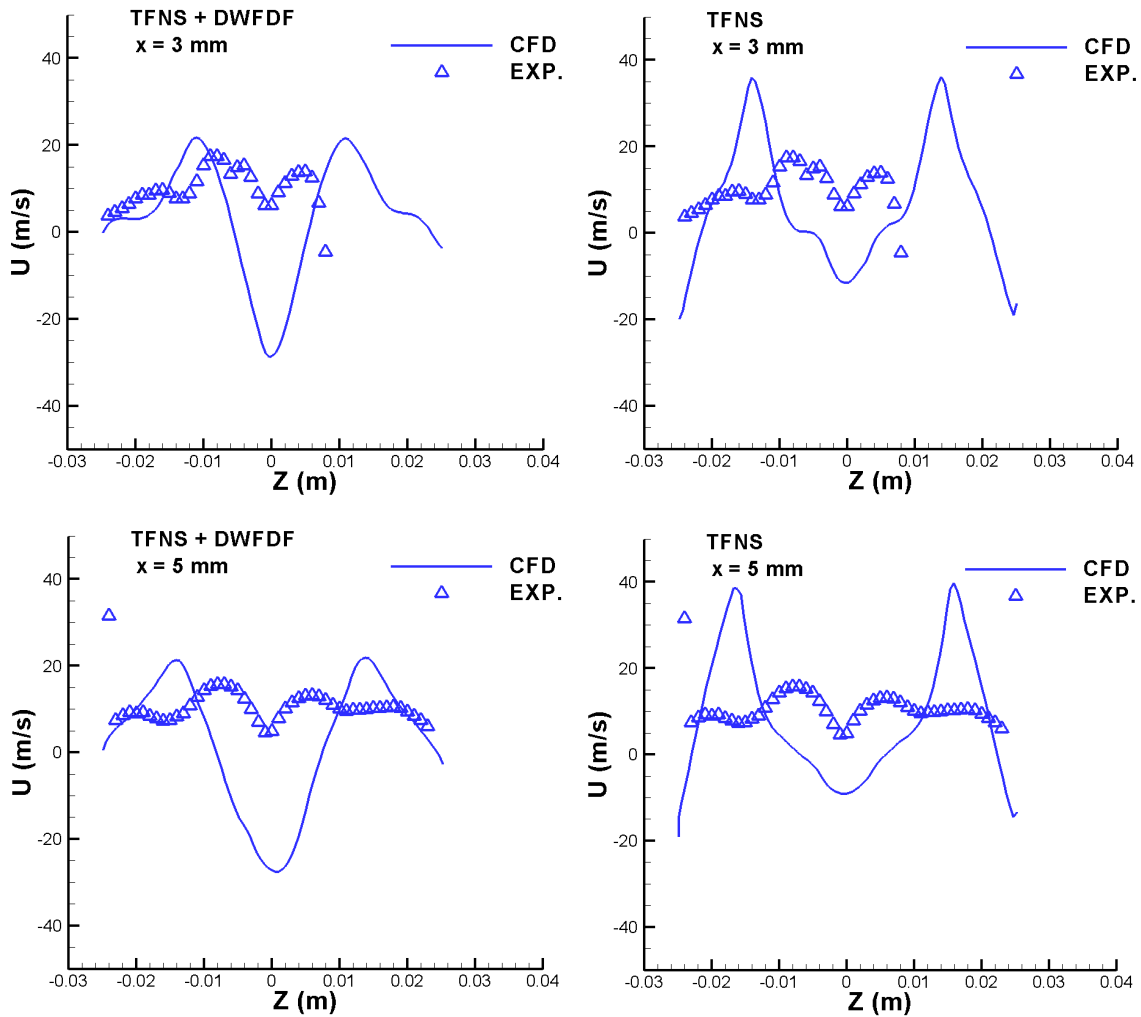


Figure 12.—Comparison of velocity component U along Z axis at downstream locations.

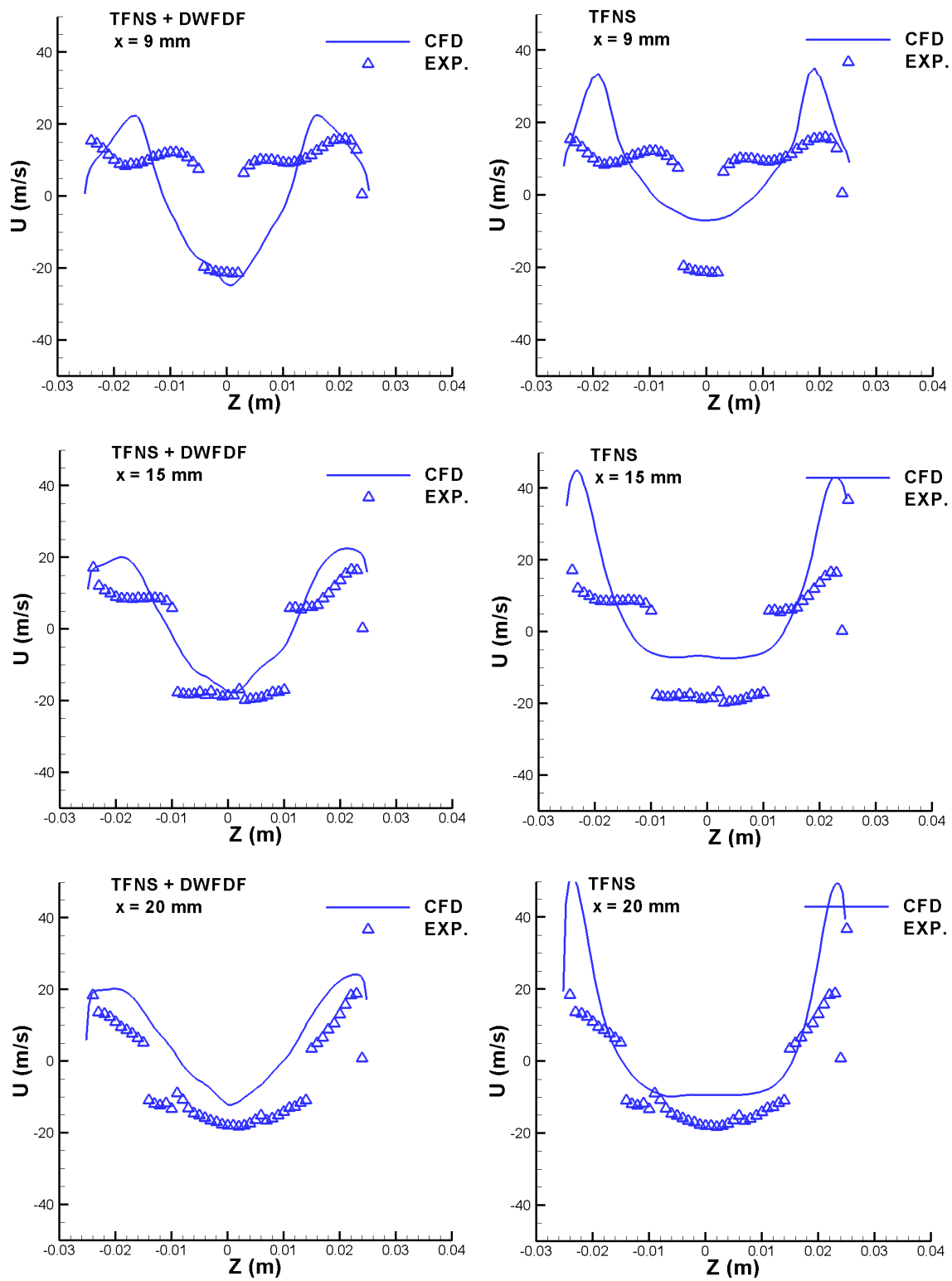


Figure 12.—Continued.

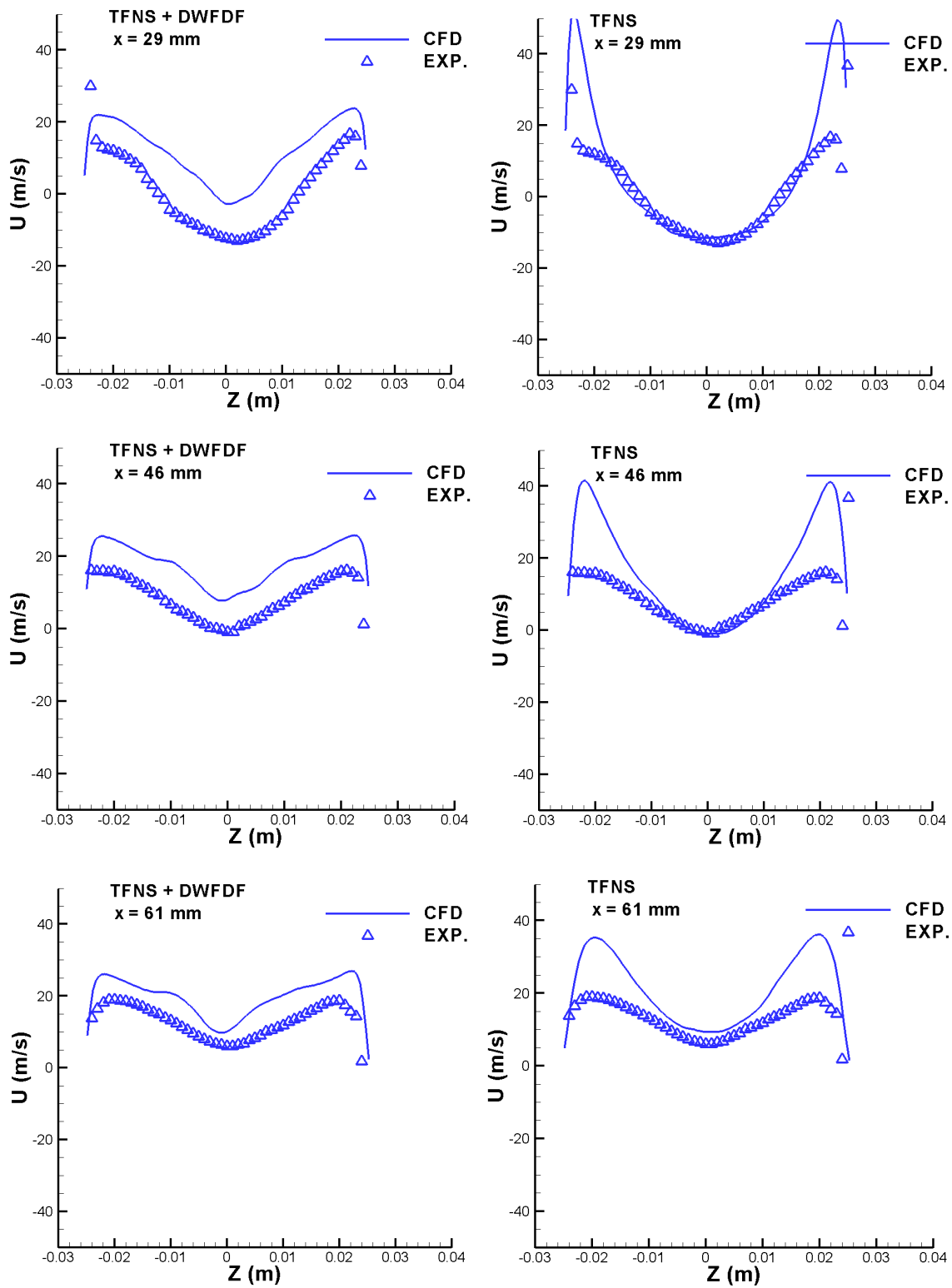


Figure 12.—Continued.

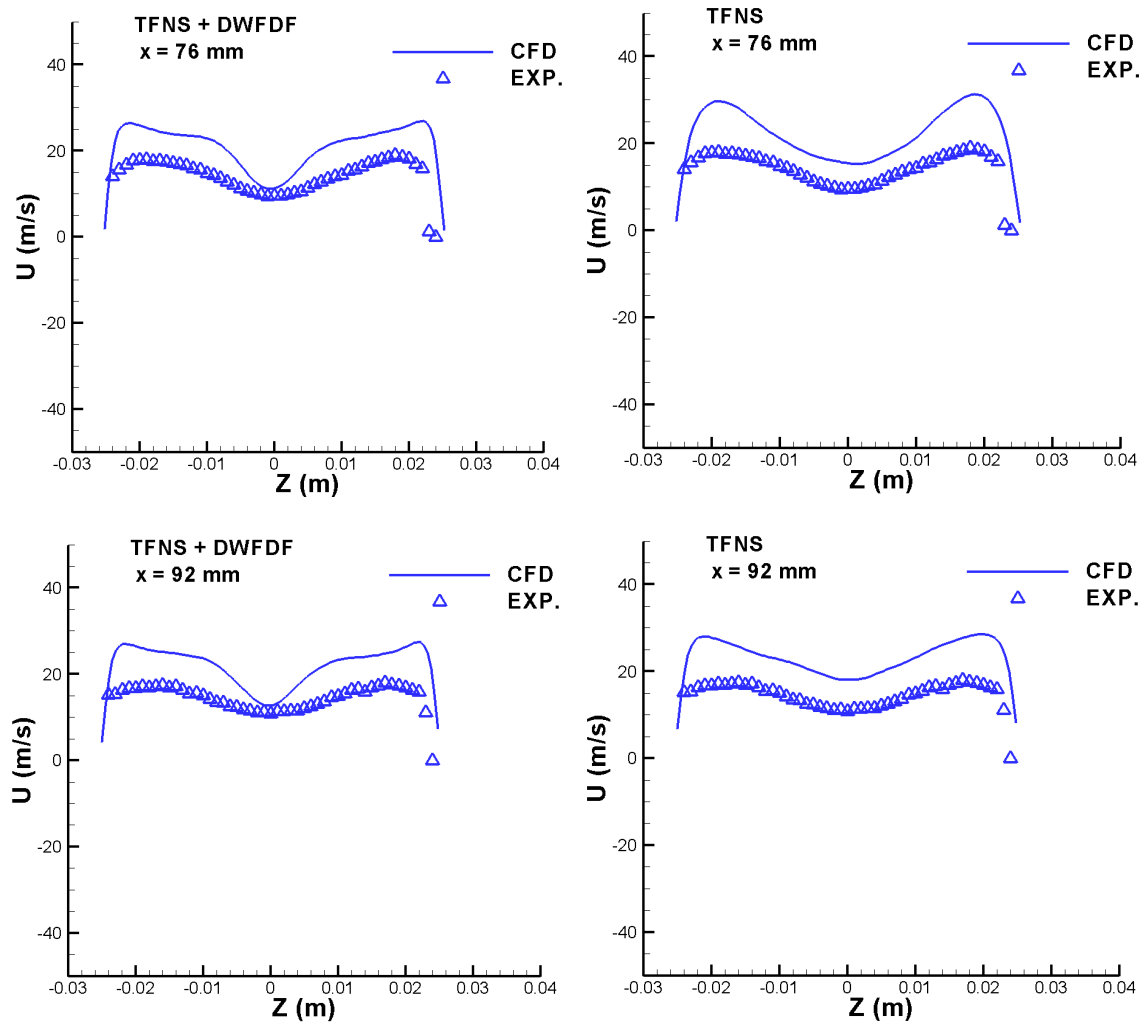


Figure 12.—Concluded.

4.5 Flow Structure and Contour Plots of Variables in the Center X-Z Plane

To reveal the simulated mean flow and flame structures, we have plotted the center recirculation zone using the iso-surface of zero axial velocity (see Figure 13), the contour plots of velocity components, vorticity magnitude, temperature, turbulent kinetic energy and species mass fractions $C_{12}H_{23}$, O_2 , CO_2 , which are shown in Figure 14, Figure 15, and Figure 16. From these figures we observe that the structures of all scalar fields simulated by TFNS with invoking DWDFD equation are quite different from the ones without invoking DWDFD equation. Also, we notice that the level of subscale turbulent kinetic energy is significantly reduced in the TFNS simulation with invoking DWDFD equation (a phenomenon often found in the simulations with the conventional or standard FDF method); however, it does not severely affect the global structure of turbulent reacting flow in our simulations due to the adoption of the new DWDFD equation, in which the time scale or frequency for the DWDFD diffusion in the sample space is not directly related to the subscale turbulent kinetic energy and its dissipation rate, instead, it is determined by the strain and rotation rate of the large turbulent flow, see Equation (59). The contours of all instantaneous variables in X-Z plane are plotted in Figure 17.

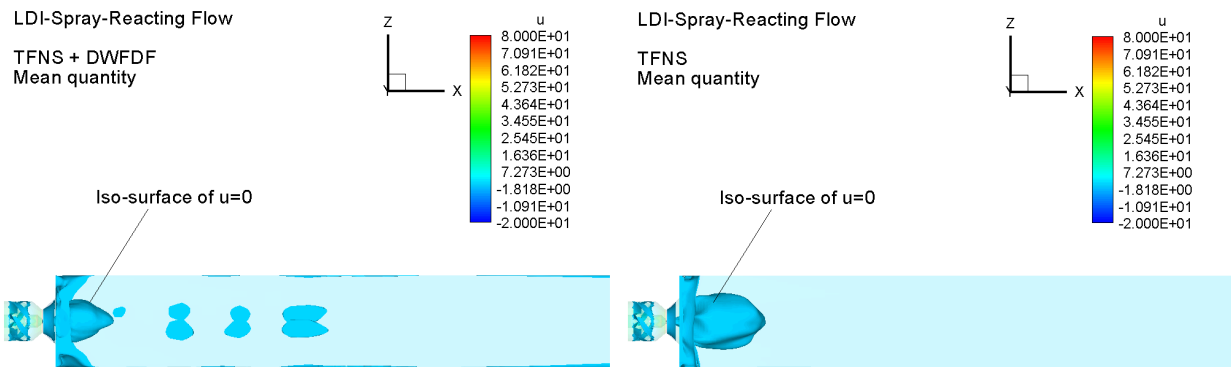


Figure 13.—Comparison of center recirculation zone.

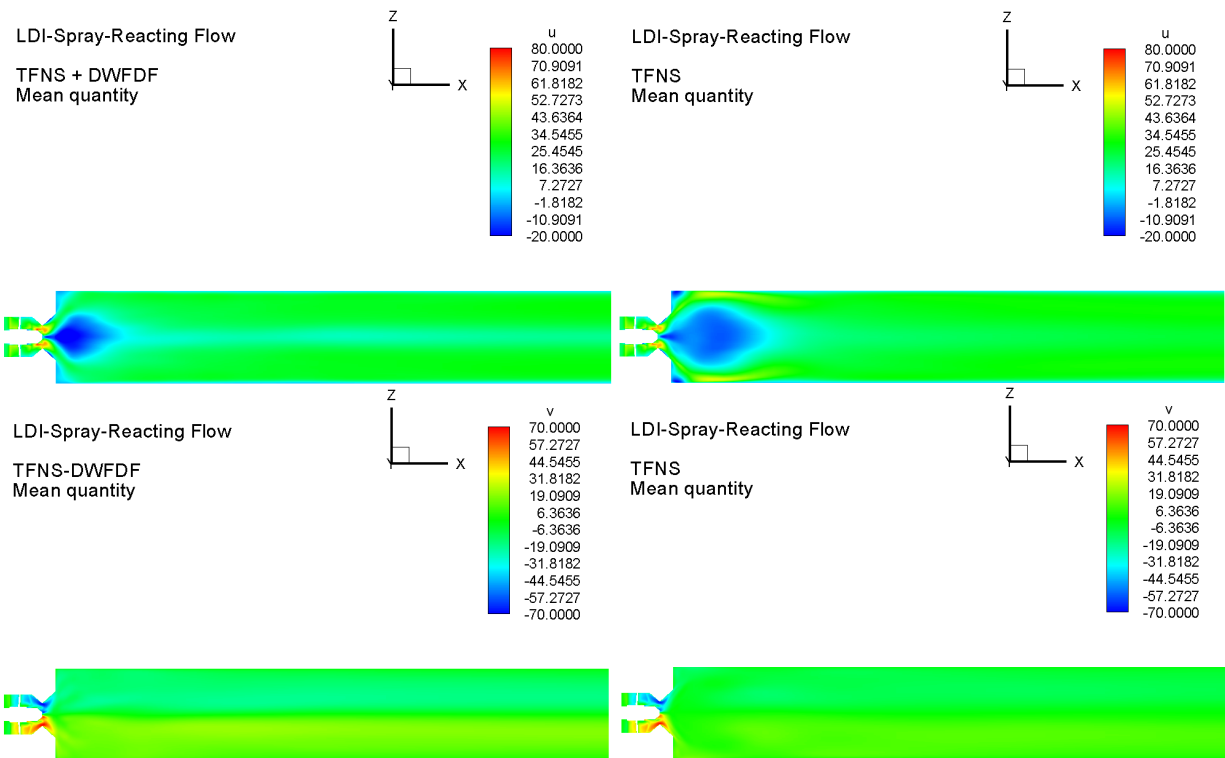
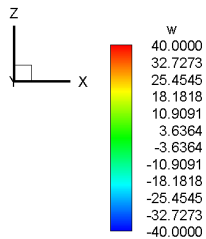


Figure 14.—Comparison of mean velocities U, V, W and vorticity contours in center plane.

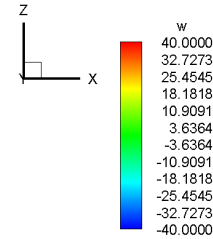
LDI-Spray-Reacting Flow

TFNS + DWFDF
Mean quantity



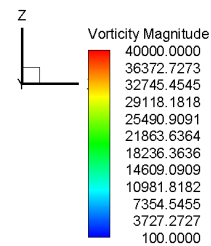
LDI-Spray-Reacting Flow

TFNS
Mean quantity



LDI-Spray-Reacting Flow

TFNS + DWFDF
Mean quantity



LDI-Spray-Reacting Flow

TFNS
Mean quantity

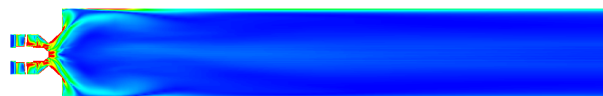
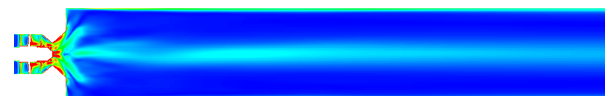
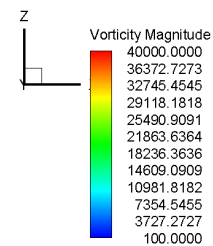
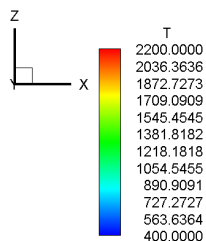


Figure 14.—Concluded

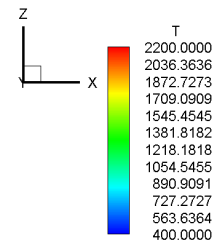
LDI-Spray-Reacting Flow

TFNS + DWFDF
Mean quantity



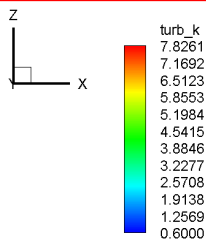
LDI-Spray-Reacting Flow

TFNS
Mean quantity



LDI-Spray-Reacting Flow

TFNS + DWFDF
Mean quantity



LDI-Spray-Reacting Flow

TFNS
Mean quantity

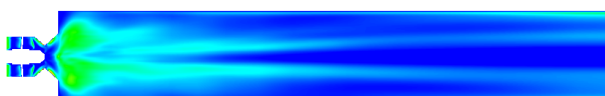
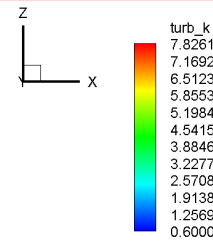


Figure 15.—Comparison of mean temperature and k contours in center plane.

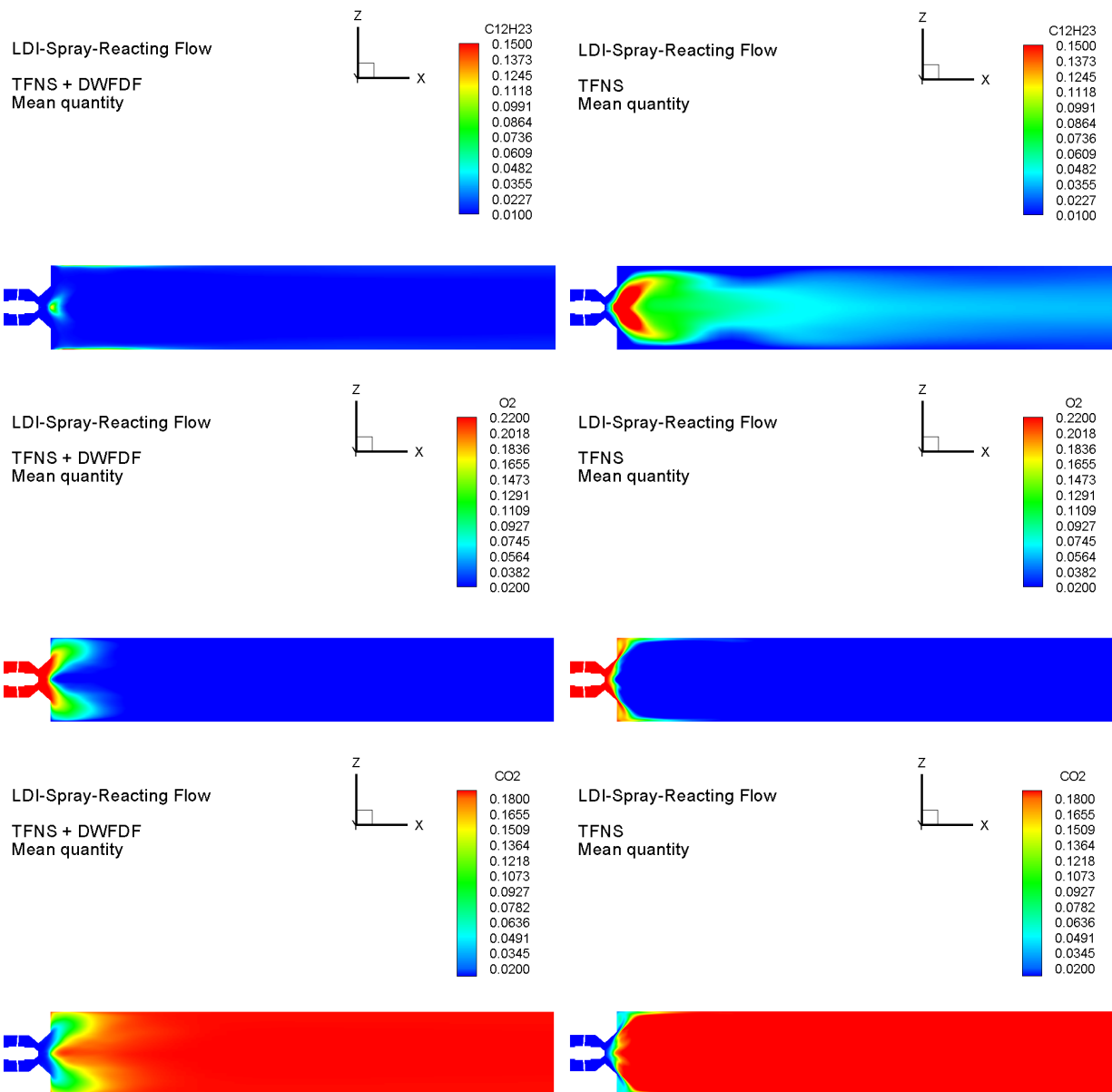


Figure 16.—Comparison of $C_{12}H_{23}$, O_2 and CO_2 contours in center plane.

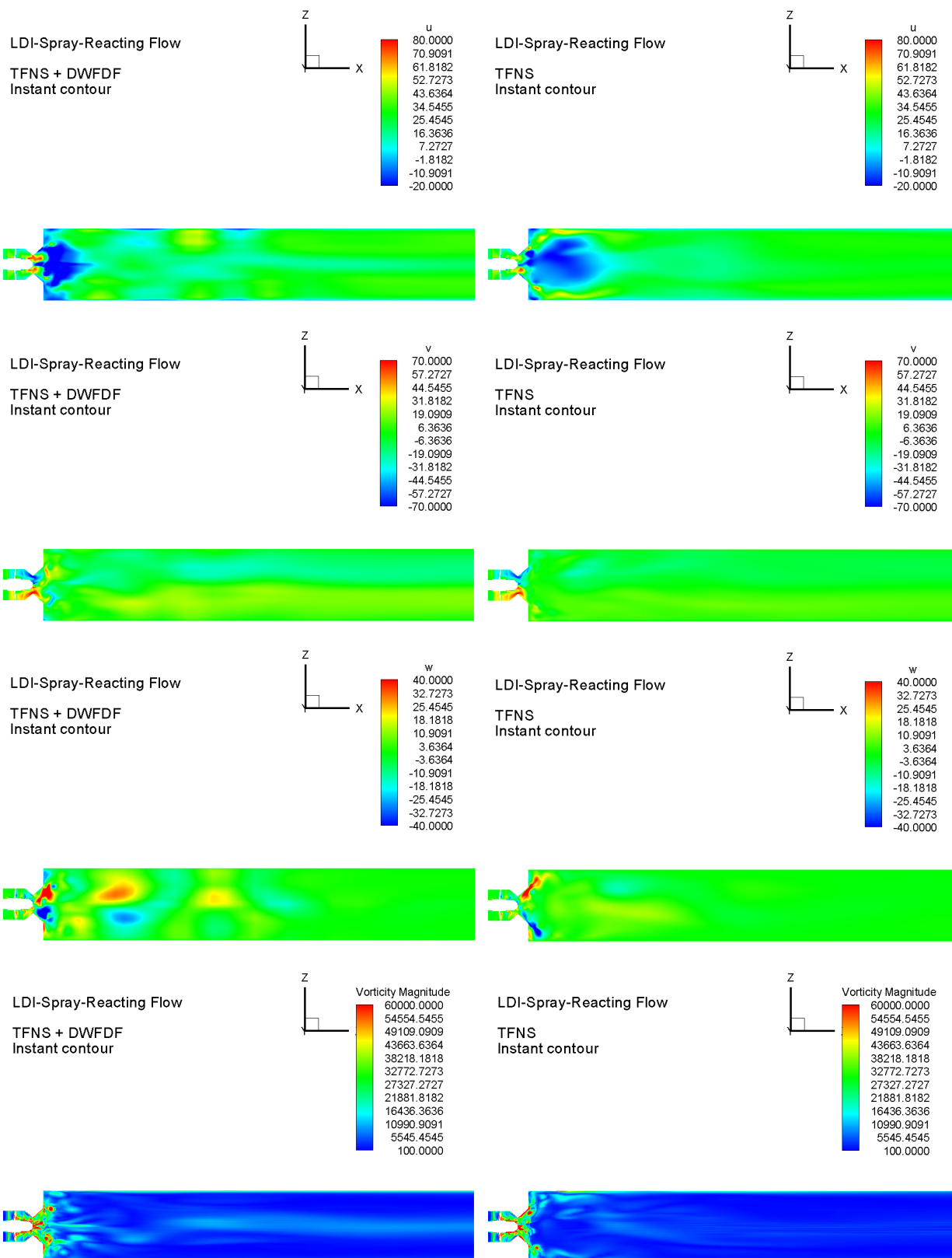


Figure 17.—Contours of instantaneous variables in X-Z center plane.

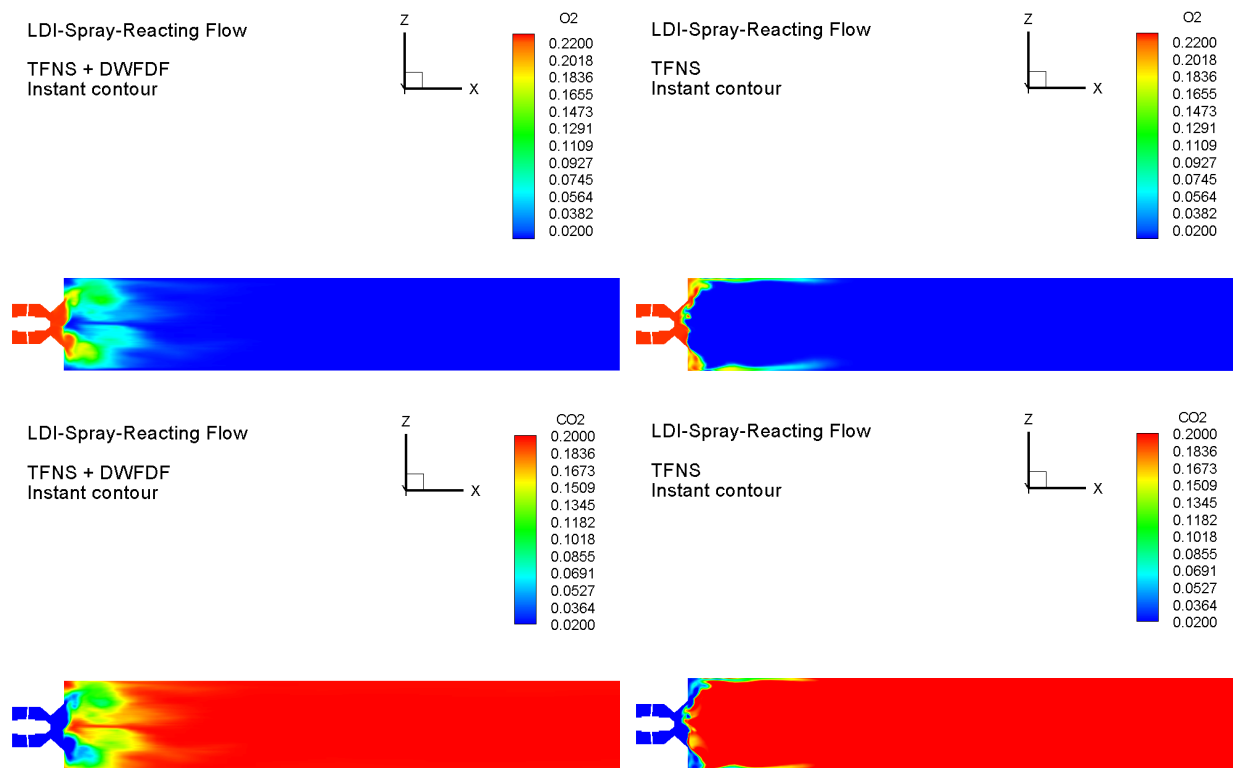


Figure 17.—Concluded.

5.0 Conclusion

The very large eddy simulations of Jet-A spray reacting flow in a single element LDI injector have been carried out both with and without invoking an Eulerian scalar DWFDF method. The NCC code is used under the same numerical setting, same computational geometry and grid resolution. In addition, the same spray model and the same chemistry kinetics are used for all the simulations. In this way, we hope to isolate and study only the effect of Eulerian scalar DWFDF method on the simulations, paying a particular attention to the simulation quality and numerical performance.

From the present simulations we have observed that there are noticeable improvements on the temperature prediction in the region of strong turbulence by using the Eulerian scalar DWFDF method. The distribution or structure of other scalar quantities appears to have a significant difference between the simulations with and without the scalar DWFDF method, and it seems to have more reasonable results by invoking the scalar DWFDF method. However, we need more reliable experimental data to evaluate and draw the conclusion. For the flow field, the effect of the scalar DWFDF method is mixed. Better predictions were observed in the axial velocity component.

As to the numerical performance, the observation is that the simulations with invoking an Eulerian scalar DWFDF method appear to have a faster convergence and more stable than the simulations without invoking Eulerian scalar DWFDF method.

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14. ABSTRACT This paper presents the very large eddy simulations (VLES) of a Jet-A spray reacting flow in a single element lean direct injection (LDI) injector by using the National Combustion Code (NCC) with and without invoking the Eulerian scalar DWDFD method, in which DWDFD is defined as the density weighted time filtered fine grained probability density function. The flow field is calculated by using the time filtered compressible Navier-Stokes equations (TFNS) with nonlinear subscale turbulence models, and when the Eulerian scalar DWDFD method is invoked, the energy and species mass fractions are calculated by solving the equation of DWDFD. A nonlinear subscale model for closing the convection term of the Eulerian scalar DWDFD equation is used and will be briefly described in this paper. Detailed comparisons between the results and available experimental data are carried out. Some positive findings of invoking the Eulerian scalar DWDFD method in both improving the simulation quality and maintaining economic computing cost are observed.					
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